

necessary to achieve vacancy supersaturation in the region of the diffusion. This can be accomplished using MeV silicon implantations.

9.8 DIFFUSION SYSTEMS AND DIFFUSION SOURCES

Regardless of the predeposition process (chemical or ion implantation) a drive-in (or redistribution) step is usually required to move the dopants in the silicon (i.e., to attain electrical activation, and reduce the implantation damage). This drive-in step is performed either in a diffusion furnace or a rapid thermal annealing (RTA) system. (These technologies are both discussed in detail in Chap. 8.) However, RTA allows dopant activation to occur using a smaller thermal exposure than can be obtained with a furnace. As a result, the use of RTA for annealing ion-implanted shallow source/drain junctions in CMOS device processing has become more popular. There are some advanced device flows that use only RTA for drive-in diffusions.

Not all fabrication processes, however, use ion implantation for dopant introduction. Some still use chemical procedures. For example, backside phosphorus gettering (Chap. 2) uses a POCl_3 source and a diffusion furnace, while bipolar base diffusions may be predeposited in diffusion furnaces sourced with boron nitride (BN) discs. Nevertheless, ion implantation is the standard technology for introducing dopants into Si wafers, and this topic is covered in Chap. 10. New technologies are still being developed for creating shallow junctions in ULSI devices, and a discussion of these follows. Older technologies for chemical diffusion of dopants into Si are covered in the 1st edition of this text (© 1986); interested readers are referred there for this information.

9.8.1 Advanced Diffusion Technologies

Advanced technologies have been studied for introducing dopants into a silicon device. These new techniques include: a) *plasma immersion ion implantation doping* (PII); b) *rapid vapor phase doping* (RVD); and c) *gas immersion laser doping* (GILD). In this section, RVD and GILD will be briefly discussed. The subject of PII is covered in Chap. 10.

9.8.1.1 Rapid Vapor Doping (RVD): Rapid vapor doping (RVD) is emerging as an alternative to ion implantation doping for some advanced applications, such as capacitor doping for DRAMs, side-wall doping in deep trenches, and even for shallow source/drain junctions in CMOS applications. Unlike vapor doping in a furnace, RVD does not depend on the formation of a doped glass layer on the surface of the wafer. For RVD, the doping proceeds directly from the gas phase into the solid. For that to occur the dopant must first be adsorbed on the silicon surface, followed by solid-state diffusion. The potential advantages of the RVD technique over ion implantation (particularly for shallow-junction applications) are that RVD does not suffer from the effects bedeviling implantation, namely: channeling, lattice damage, or wafer charging.

Rapid vapor doping uses rapid thermal processing (RTP) to quickly and uniformly heat the wafer to the desired temperature while the wafer is exposed to a gaseous dopant source. The precise control of the gas flow and dilution are necessary to ensure a uniform dopant concentration across the wafer surface. The final dopant surface concentration (C_s) and junction depth (x_j) depend on the gas phase concentration of dopant and the duration and temperature of the RTP treatment. The gas phase concentration is controlled by diluting the source gas (e.g., phosphine) with a hydrogen carrier gas. There are some disadvantages of RVD, such as: a) a relatively high thermal budget is required for the surface reaction and solid-state diffusion to get the dopants into the silicon; and b) "hardmasks" are required for selective doping.

There have been reports describing the RVD fabrication of shallow boron junctions from vapor sources. Kiyota *et al.*, reported forming ultra-shallow boron junctions by flowing B_2H_6 in H_2 at $900^\circ C$ for 30 sec.⁴⁹ This process resulted in a junction depth of 30 nm and a surface concentration of $5.8 \times 10^{19} \text{ cm}^{-3}$. This level of doping is adequate for fabricating base regions in bipolar devices or the source/drain extensions in CMOS devices. Short-channel CMOS devices produced using RVD showed improved performance over devices produced by conventional ion implantation.⁵⁰ Similar studies using phosphine (PH_3) diluted in hydrogen at $900^\circ C$ reported junction depths <100 nm and surface concentrations between 3.0×10^{18} and $1.3 \times 10^{19} / \text{cm}^3$.⁵¹

9.8.1.2 Gas Immersion Laser Doping (GILD): The origins of GILD technology extend back more than 15 years, when lasers were first used to locally melt silicon immersed in a doping gas (such as PF_5 or BF_3).^{52,53} The technology has been refined since that time, and it is now possible to fabricate devices using GILD technology. The basis of GILD technology is to shine high energy density ($0.5\text{--}2.0 \text{ J/cm}^2$) *eximer laser* light (308 nm) for a short pulse time (20–100 ns) onto a silicon wafer immersed in a dopant gas phase. The energy is absorbed into the first 10 nm of the silicon surface, where it dissipates by melting the surface layer. The thin melted layer absorbs and dissolves the dopant atoms directly from the gas phase. Since the diffusivity of the dopants in the liquid phase is about 8 orders of magnitude faster than in the solid phase, the dopants rapidly and uniformly diffuse throughout the molten layer. When the laser power is turned off, the thin molten layer epitaxially recrystallizes (freezes). During recrystallization the dopant is incorporated into the silicon lattice on substitutional sites. Consequently, the majority of the dopant is activated immediately after cool down and no further anneal is required. The liquid-to-solid transformation occurs at an extremely high rate ($> 3 \text{ m/s}$) and it is possible for the amount of active dopant incorporated in the silicon to exceed the equilibrium concentration (supersaturation). As long as the wafer is not subjected to subsequent elevated temperature processing, the excess dopant will stay in solution.

Since the time that the wafer is exposed to the high-energy laser beam is short, the bulk of the wafer remains cool and little or no solid-state diffusion occurs. As a result the dopant is confined only to the molten region and any dopants that were previously introduced into the silicon remain unperturbed. The depth of the junction is controlled by the depth of the molten silicon, which depends on the energy density and pulse time of the laser treatment.

Since the concentration of the dopant is uniform throughout the “diffused” region the concentration profile tends to be more box-like rather than *erfc* or Gaussian. Consequently, the profile gives an abrupt junction. Figure 9-19 shows the diffusion profile after a GILD of phosphorus in a *p*-type substrate. The box-type profile is apparent. A 30 ns pulse results in a junction depth of 30 nm with a surface concentration $4 \times 10^{20} / \text{cm}^3$. As the pulse time increases the junction depth gets deeper.

A major innovation towards making GILD a production-worthy technology was the introduction of *projection-GILD* or *P-GILD*. This technology utilizes a step-and-repeat camera, similar to those described for projection lithography in Chap. 13. Eximer laser light is shined through a dielectric mask. The light from the mask is demagnified (e.g., a 4x reduction), focused, and projected onto the wafer. The wafer is stepped after each field of the mask is exposed (or melted, in this case). The amount of doping incorporated into the layer increases as the number of laser exposures increase, while the depth of the junction increases with the increase in the energy of each pulse. The dopant is incorporated only in the regions that are melted (i.e., only beneath the regions of the mask that transmit the laser light).

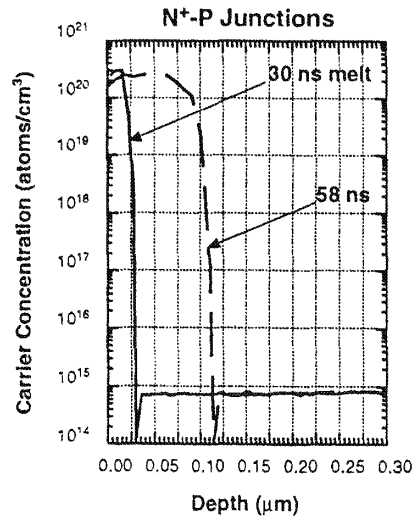


Fig. 9-19 Spreading resistance profile (SRP) for a phosphorus doped P-GILD formed in a *p*-type doped substrate. Note that x_j increases with surface melt time and the diffusion profile forms a "box" type profile with no anomalous tail.⁵³

9.9 MEASUREMENT TECHNIQUES FOR DIFFUSED (AND ION-IMPLANTED) LAYERS

The diffusion coefficient D is experimentally determined from the concentration profile in the silicon subsequent to chemical predeposition (or ion implantation) and drive-in. In order to determine accurate values of D , reliable measurements of the junction depth, sheet resistance, and diffusion profile must be feasible. Sheet-resistance measurements have become the standard method for "in-line" monitoring of diffusion processes in IC production facilities. These measurements are performed immediately after a diffusion step. In this section some of the important measurement techniques for determining sheet resistance and doping profiles are described.

9.9.1 Sheet Resistance Measurements

The *sheet resistance*, R_s of a diffused layer is the resistance exhibited in a square (i.e., a region of equal length and width) of that layer, which has a thickness x_j (junction depth). The value of R_s is expressed in units of ohms/sq (Ω/sq), and is related to the *average resistivity* ρ of a diffused layer by:

$$R_s (\Omega/\text{sq}) = \rho (\text{ohm-cm})/x_j (\text{cm}) \quad (9.48)$$

The layer (or film) resistivity is a material property that depends on the number of free carriers and the mobility of these carriers. The average resistivity ρ is found from:

$$\rho = \left[q \int_0^{x_j} \mu(C_A) C_A(x) dx \right]^{-1} \quad (9.49)$$

where q is the charge on a carrier $\mu(C_A)$ is the carrier mobility (which is a function of the carrier concentration), and $C_A(x)$ is the diffusion profile.

The value of R_s is readily obtained by measuring the resistance of the diffused layer using the *4-point probe technique*.⁵⁴ Figure 9-20 shows the co-linear probe arrangement that is the basis for the ASTM standard,⁵⁵ which is the standard for measuring R_s . To make this measurement a current, I , is forced between the outer two probes, and the voltage drop, V , is measured between the two inner probes. When all of the probes are equally spaced, the resistivity is given by:

$$R_s = 2\pi sF(V/I) \quad (9.50)$$

where s is the probe spacing, and F is a correction factor (that arises from the fact that the sample is not semi-infinite, but has a finite thickness and diameter).⁶⁴ When the sample thickness t is small, relative to the probe spacing (as in the case of a diffusion, where $t = x_j$), then Eq. 9-50 can be rewritten as:

$$\rho = 4.532t\left(\frac{V}{I}\right) \quad \text{or} \quad R_s = \frac{\rho}{t} = 4.532\left(\frac{V}{I}\right) \quad (9.51)$$

There is an additional set of correction factors related to the finite diameter of the wafer and the effect of the probes being close to the edge of the wafer. The correction factor is 1 if the probes are at least 3x their spacing from the wafer edge. When the probes are closer to the edge, the correction factor decreases to a value of 0.5–0.7, depending on the orientation of the probes to the wafer edge. The factors are listed in Ref. 64. For a standard probe spacing of 0.0625 inches, the probes need at least 4.7 mm from the wafer edge in order not to require a correction factor. To prevent erroneous readings the probe spacings must be accurately known, and if they are not equal, that must also be taken into account in the correction factor.

The sheet resistance measurement is first performed with the current in the forward direction, and then in the reverse direction (in order to minimize errors due to thermoelectric heating and cooling effects). The two (V/I) readings are averaged. The measurements should also be made at several current levels, until the proper level is found. That is, if the current is too low, the values of the forward and reverse readings will differ, while if it is too high, I^2R heating will cause the measured reading to drift with time. The ASTM standard also recommends best current levels, which depend on the resistivity range of the diffused layer. The amount of pressure applied to the probes during measurement is also important, since excessive pressure can drive the probes past the junction, while too little pressure results in poor electrical contact to the sample.

Automated 4-point probe equipment is currently available from several vendors. The equipment is capable of measuring the sheet resistance in numerous places on the wafer. The

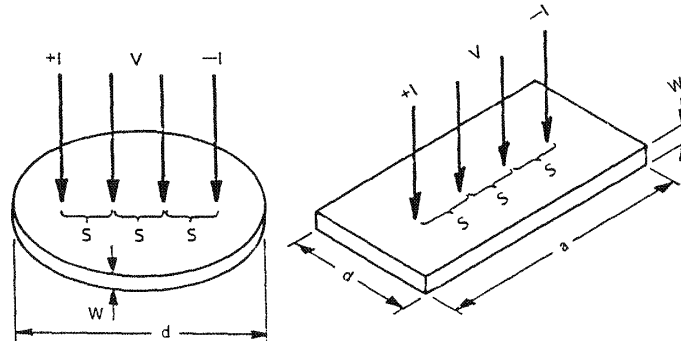


Fig. 9-20 Co-linear four-point probe arrangement for the measurement of resistivity.

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system has a built-in algorithm to calculate the sheet resistance at these points and to use the appropriate correction factor for each position. The data can be presented in a graphical format using a *contour map* of resistivity. In this way the process engineer can look for process variations that are wafer dependent. The program can also calculate and depict statistical information about the sheet resistance variation. Such tools are used for in-line process control in many wafer fabs.

It is possible to estimate the doping profile of a diffusion using the *differential sheet resistivity* technique. In this technique, the sheet resistivity is measured initially and then again after a small amount of the silicon surface is removed. Anodic oxidation, followed by an etch of the anodic film, is used to control the amount of silicon removed in each step. The sheet resistivity will increase as dopant is removed, since the amount of doping is decreasing and the thickness of the diffused layer is decreasing with each step. The rate of the increase in R_s depends on the resistivity profile shape. The resistivity depends on the dopant concentration and the carrier mobility. If the mobility is known for each value of resistivity, the carrier concentration profile can be obtained with this technique. Note that the differential-sheet-resistivity method is tedious, and is only used in special cases where other profiling techniques are not available.

9.9.2 Capacitance-Voltage (C-V) Measurements

The carrier concentration profile can be measured directly within a diffused region by using the C-V technique. The use of C-V measurements to determine the diffusion profile is predicated on the measurement of the reverse bias capacitance of an n^+/p or p^+/n junction as a function of voltage. The capacitance of a junction is given by:

$$C(V) = \left[\frac{q\epsilon_{Si}C_A}{2} \right]^{1/2} \left[V_{bi} \pm V_R - \frac{2kT}{q} \right]^{1/2} \quad (9.52)$$

where ϵ_{Si} is the permittivity of silicon, C_A is the substrate doping concentration, V_{bi} is the built-in potential of the junction, and V_R is the applied reverse bias voltage.

The technique requires the formation of a very shallow n^+ or p^+ diffusion over the surface of the diffused layer of interest. The doping in the heavily doped region must be more than 100 times that in the lightly doped region (where the profile is measured) for the technique to work. The capacitance is measured while applying a variable reverse dc voltage to the junction. The instantaneous value of C_A is then calculated from Eq. 9-52. The depth at which C_A is measured is obtained from the value of the applied reverse voltage, assuming the distance equals the depletion width of a one-sided junction. If those conditions hold, the depth of the measurement is given by:

$$x = \sqrt{\frac{2\epsilon_{Si}(V_{bi} + V_R)}{qC_A}} \quad (9.53)$$

The major limitation of this technique is that the initial values of C_A that are measured are at least as deep as the value of x_j for the n^+ or p^+ diffusion plus the zero-bias depletion width (which extends into the substrate). The depth of the profiling is limited to the reverse breakdown voltage of the junction. Therefore, the C-V technique has little value for determining the doping profile in shallow junctions. The technique also falls short when abrupt profiles are measured, since fictitious tails are often observed near the steep edge.⁵⁶

9.9.3 Spreading Resistance Profiling (SRP)

The use of *spreading resistance* SR (i.e., the resistance associated with the divergence of the current lines emanating from a small-tipped electrical probe that is placed onto the silicon), was first proposed by Mazur and Dickey for measuring the thickness of diffused or epitaxial layers, and establishing the impurity profile for these structures.⁵⁷ The technique is referred to as *spreading resistance profiling* (SRP). In this technique, the SR of a reproducibly formed point-contact is measured. This can be accomplished by using one, two, or three probe configurations. The two-probe method has met with the most success on commercially available equipment. SR measures only the electrically active dopant concentration, and other techniques, such as SIMS, are needed if the total (active + inactive) concentration profile is required.

To make spreading resistance measurements, a known current is applied between the probes, and the voltage drop is measured across these probes to obtain a spreading resistance ($R_{SR} = V/I$). Most of the voltage drop occurs at a distance that is only a few times the probe radius, and therefore the value of R_{SR} is measured in a very small volume of silicon immediately under the probe. In the two probe method, the Si resistivity ρ is related to the R_{SR} by the relationship:

$$\rho = 2 R_{SR} a \quad (9.54)$$

where a is an empirical quantity which is related to the effective electrical contact radius (it is not however the probe tip radius). The value of a is determined by measuring R_{SR} on a well-characterized material of known resistivity. An ASTM Standard has been developed for conducting SR measurements, and the reader is referred to this reference for details.⁵⁸

In order to use spreading resistance the probe tips must be well conditioned. This is achieved by stepping the probes at least 500 times on a silicon substrate that has been ground with fine grit. The probe tips must also be calibrated to obtain the empirical value of a . This is best done on a wafer that has a well-documented resistivity (determined using a more direct technique). It is important that the surface of the calibration wafer and the surface of the unknown sample be identically prepared.

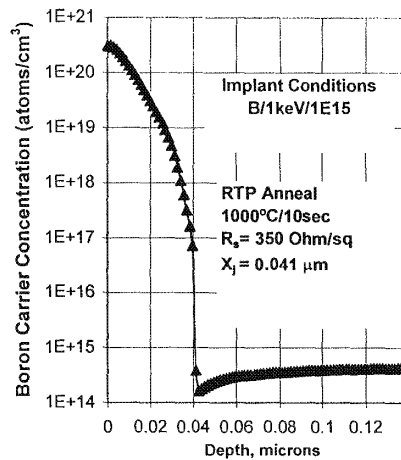


Fig. 9-21 Spreading resistance profile measurement showing the capability of measuring very shallow junctions. Courtesy of Applied Materials

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The main use of SR is to determine doping profiles of diffused or epitaxial layers. This is accomplished by angle lapping the wafer and then making SR measurements along the length of the lapped surface. Knowing the angle of the taper gives the depth as a function of distance from the surface. The same precautions used to lap a wafer for junction depth measurements (see next section) must be obeyed when beveling a specimen for SR measurements, including the use of the laser measurement to determine the angle. Elaborate correction techniques and correction factors (CF) have been developed to convert the values of R_{SR} into carrier concentration values, particularly in multilayer samples. The values of the CFs depend on the nature of the layer and the proximity of the measurement to the junctions.

By beveling the sample to extremely low angles (<0.05 degrees), it is now possible to perform SRP on very shallow junctions. The skill required to accurately make these measurements is restricted to a few commercial laboratories.⁵⁹ Fig. 9-21 shows a SR profile for a shallow junction boron diffusion, with an x_j of only 30 nm. The most difficult part of the measurement is determining where the top surface ends and the bevel starts. Depositing a layer of polysilicon on the top surface can aid in finding where the bevel begins.

9.10 JUNCTION DEPTH MEASUREMENTS: PHYSICAL TECHNIQUES

9.10.1 Angle Lap and Stain

The *angle-lap and stain method* is effective for determining the depth of some *pn* junctions, and the test method is available in ASTM Standard Test Method F-110-84.⁶⁰ The method works well on relatively deep, highly-doped junctions, but is not accurate for shallow junctions. Wu *et al.* have reported that the accuracy of this technique can be significantly improved (to ± 20 nm of the true metallurgical junction), if the proper lapping and staining precautions are taken.⁶¹

The angle-lapping technique requires the grinding of a small angular bevel on the silicon wafer. This is accomplished by mounting the wafer on an angle block, and moving the assembly over a flat glass onto which a lapping-compound slurry has been poured. To obtain small angles ($\leq 1^\circ$) of good quality, the following practices should be followed:

1. The angle-lap assembly should be massive, to eliminate rocking during the lapping process. Small pieces of silicon affixed to the bottom of the holder, where they act as runners, are found to be helpful in minimizing the rocking, as well.
2. A slurry consisting of the lapping compound (alumina of $\leq 0.3 \mu\text{m}$ particle size, mixed with water) is used. The slurry should be changed often to keep it free from dirt and Si chips.
3. Any metallization on the wafer surface should be removed prior to lapping, since it smears when lapped, and will interfere with the subsequent staining process.
4. If the region of interest does not have a reasonably thick (>300 nm) protective oxide or nitride layer, edge rounding can occur. This can make it difficult to locate the position of the surface with certainty. Thus, it is good practice to chemically deposit ~ 500 nm of low temperature silicon dioxide onto such surfaces prior to lapping.

After lapping has been performed (which brings the junction to the surface), a staining solution is used to delineate either the *n*-type area or the *p*-type area. One such stain consists of a copper sulfate (CuSO_4) solution for staining the *n*-region. The staining occurs as a result of the following events: a) a drop of CuSO_4 is dispensed onto the junction; b) at the same time the junction is illuminated by an intense light source which causes it to become forward-biased;

Chapter 10

ION IMPLANTATION FOR ULSI

Ion implantation is a process in which energetic, charged atoms (or molecules) are directly introduced into a substrate. In ULSI fabrication, ion implantation is primarily used to add dopant ions (most often selectively) into the surface of silicon wafers. Acceleration energies for CMOS doping applications range between 0.2 keV (for shallow junctions such as source/drain extensions) to ≈ 2 MeV (for multiple-well doping). The superiority of ion implantation over chemical (diffusion) doping methods has enabled implantation to replace diffusion doping for almost all planar doped structures (i.e., one exception involves the doping of deep trench sidewalls, in which impurities are diffused into the Si from doped CVD SiO_2 films).

Ion implantation is superior to chemical diffusion for introducing dopants for the following reasons:

1. Ion species can be implanted with high accuracy over many orders of magnitude of doping levels (whereas dopant control by diffusion is far less exact).
2. Depth profiles of the implanted species can be established by controlling ion energy and channeling effects. This capability can be extended to produce the depth profiles needed in complex applications by using multiple-energy implants.
3. By using polymer-based photoresist patterns as the masking material, dopants can be introduced into selected regions of the wafer surface at near-room temperatures.
4. Both p - and n -type dopants (with a variety of activation and diffusion characteristics) can be implanted into Si.
5. The crystalline structure of implant-damaged Si can be recovered through subsequent thermal annealing cycles.

In this presentation, the physical mechanisms which determine implanted atom profiles will first be discussed. A comparison between theoretical models and experimental observations (i.e., to illustrate how closely actual implantation profiles match the profiles predicted by the models) will then be provided. Next, a description of ion implantation systems is undertaken (including safety aspects and operational limitations). This is followed by a presentation of the methods used to monitor and evaluate various aspects of ion implantation, including: a) implantation doses; b) implantation dose uniformity across a wafer; c) implantation profiles; d) implantation damage; and e) the degree to which damage is removed (and/or remains) after annealing. Finally a group of topics relating to practical aspects and specific applications of ion implantation processes for CMOS transistors is discussed. Table 10-1 lists some of the important applications of ion implantation in ULSI.

Note that this chapter was revised by Dr. Michael Current.

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Table 10-1 ION IMPLANTATION APPLICATIONS IN ULSI CMOS

Junction Formation (Used to fabricate both MOS and bipolar devices)	Miscellaneous Process Applications
CMOS Fabrication (see Vol. 2 of this series) - Threshold Voltage Control/Adjustment - Channel-Stop Implantation - Source/Drain Formation - Well Formation - Punchthrough Stopper Implantation - Graded Source and Drain Formation	- Backside Damage Layer Formation for Gettering (see Chap. 2) - High-Energy Implantation to Form Buried Layers for Gettering - Ion Beam Mixing to Promote Silicidation Reactions - Buried Insulator Layer Formation (Chap. 7 and Vol. 2 of this series) - Nitrogen Implantation into Poly-Si Gates to Reduce Boron Diffusion
Bipolar Fabrication (see Vol. 2 of this series) - Predeposition - Base Formation Implantation - Arsenic-Implanted Poly-Si Emitter - High Value Resistor Formation Implantation	- Polysilicon Resistor Formation - High Energy Implantation to Form Buried Collectors - Emitter Formation Implantation
Formation of Silicon-on-Insulator Materials - High Dose Oxygen Implantation (SIMOX - see Ch. 7) - High Dose Hydrogen Implantation (Smart-Cut- see Ch. 7))	

It is useful to begin the discussion with a definition of *implantation dose*. The ion beam current in implanters ranges between about 1 μA and 30 mA, depending on the implant species, energy, and type of implanter. (Implanters used for oxygen implantation for the formation of SIMOX materials have beam currents in the range of 50–100 mA.) The number of implanted ions per unit area is termed the *dose*, ϕ . Typical doses range from 10^{11} – 10^{16} atoms/cm². The dose (in atoms/cm²) is related to beam current I (in amperes), beam area A (in cm²), and implantation duration, t (in sec) by:

$$\phi = \frac{I t}{q_i A} \quad (10.1)$$

where q_i is the charge per ion (normally equal to one electronic charge = 1.6×10^{-19} coulomb).

10.1 ADVANTAGES (AND PROBLEMS) OF ION IMPLANTATION

10.1.1 Advantages

1. The *most important advantage* is the ability to more precisely control the number of implanted dopant atoms into substrates (e.g., with a repeatability and uniformity of better than $\pm 1\%$). For dopant control in the concentration range of 10^{14} – 10^{18} atoms/cm³, ion implantation is clearly superior to conventional chemical deposition techniques.
2. Implanted impurities are introduced into the substrate with less *lateral* distribution than from diffusion doping processes. The reduced lateral impurity penetration allows devices to be fabricated with smaller feature sizes.
3. Mass separation by the ion implanter allows elemental selection for dopant beams, even if the source materials contain a mixture of elements.

4. A single ion implanter can be used for a variety of implant species. There is a risk of cross contamination by other species used in the implanter through sputtering and vapor transport, but newer generation implanters minimize this problem through innovative equipment designs.

5. Ion implantation can inject dopant atoms into a semiconductor by implantation through a thin surface layer (e.g., SiO_2). The surface layer can also serve as a protective screen against contamination by metals and other dopants during the introduction of the desired impurities.

6. The distribution of implanted ions in silicon can be modeled and predicted to a high degree of accuracy for most dopants and transistor materials. This is a tremendous advantage in new device and process development.

7. Complex-doping profiles can be produced by superimposing multiple implants having various ion energies and doses.

8. Under some implantation conditions either highly abrupt or graded junctions can be formed.

9. A variety of materials are suitable for creating masks to keep ions from being implanted into unwanted regions. The masking layer prevents ions from being introduced into regions under the mask (except near the mask edge). Lateral scattering effects do occur as a result of the ion implantation process, but are smaller than lateral diffusion distances.

10. Ion implantation is a near-room-temperature process, allowing materials such as polymer-based photoresist to routinely be used as implant-mask layers.

11. The inherent purity of processing under high vacuum reduces problems from a variety of contamination and defect causing mechanisms.

12. The parameters that control an ion implantation process are amenable to automatic control for beam setup, implantation, and cassette-to-cassette wafer motion.

10.1.2 Problems/Limitations of Ion Implantation

1. Ion implantation causes damage to the material structure of the target (i.e., the wafer). In crystalline targets (e.g., single-crystal Si wafers), crystal defects and even amorphous layers are formed. To restore the wafer to its pre-implantation condition, thermal processing after implantation must be performed. In some cases, significant implantation damage cannot be removed.

2. The maximum implantation depth achievable with conventional implanters is relatively shallow ($\approx 1 \mu\text{m}$).

3. The lateral distribution of implanted species (although smaller than lateral diffusion effects), is not zero. This is a fundamental limiting factor in fabricating some minimum sized device structures, such as the electrical channel length between source and drain in self-aligned MOSFETs.

4. Throughput is typically lower than diffusion doping processes. High implantation doses may require undesirably long implantation times, depending on the implanted species and equipment design and operation.

5. Ion implanters are complex machines, among the most sophisticated systems in the wafer fab. In order to be effectively utilized they must be conscientiously operated, monitored, and maintained by well-trained personnel.

6. Ion implantation equipment contains many potential safety hazards to the personnel who operate or service the machines (e.g., high voltage, radiation) and toxic gases). To minimize the

likelihood of accidents from operating and especially maintaining such equipment, careful safety procedures must be established and strictly followed.

7. Some older-style implanters use diffusion pumps in the beam column, and this will lead to organic chemical contamination due to oil backstreaming. The effects of such contamination are described in Chaps. 3 and 5.

10.2 IMPURITY PROFILES OF IMPLANTED IONS

In order to benefit from the ability to control the number of impurities implanted into a substrate, it is necessary to know where the implanted atoms are located after implantation (i.e., it must be possible to predict the *depth distribution*, or *profile* of the as-implanted atoms). For example, this information is necessary for selecting appropriate doses and energies when designing a fabrication process sequence for new or modified integrated circuit devices. What is needed to make accurate predictions of implantation profiles is a theoretical model (or models) based on the energy interaction mechanisms between the impinging ions and the substrate. In this section the topic of how such theoretical models have been developed, and under what conditions they provide accurate predictions of implantation profiles, will be addressed. Figure 10-1 outlines the evolution of the models developed for determining implantation profiles and indicates the conditions under which they can be used to provide useful predictions.

Despite the fact that the derivation of the models is quite mathematical and complex, the scope of this text is limited to a more qualitative discussion. Even on a largely qualitative level such a presentation is valuable. That is, it provides the reader with an appreciation of the intellectual underpinning of ion implantation profile prediction, and also serves as an introduction to other physical mechanisms associated with ion implantation. These include channeling effects during implantation, substrate damage from implantation, and recoil effects that occur when implantations are done through thin layers present on the substrate surface. Readers interested in gaining a deeper and more quantitative understanding of implantation profile models can refer to references given at the end of the chapter. Some are comprehensive surveys,^{1,2} while others are papers in which the models were originally published (and which thus discuss more fully the assumptions underlying the model, and details of the derivations and associated calculations).^{3,4,5}

10.2.1 Definitions Associated with Ion Implantation Profiles

As energetic ions penetrate a solid target material they lose energy due to collisions with atomic nuclei and electrons in the target, and eventually come to rest. The total distance that an ion travels in the target before coming to rest is termed the *range*, R . As a result of the collisions between the ions and the target material nuclei, this trajectory is not a straight line (and in fact, the value of the total distance traveled is not even the quantity that is of highest interest). What is of greater interest than R is the projection of this range on the direction parallel with the incident beam, since this represents the penetration depth of the implanted ions along the implantation direction. This quantity is called the *projected range*, R_p (Fig. 10-2a). As the number of collisions and the energy lost per collision experienced by the penetrating ion are random variables, ions having the same initial energy and mass will end up spatially distributed in the target. An average ion will stop at a depth below the surface given by R_p . Some ions, however, undergo fewer scattering events than the average, and come to rest more deeply into the target. Others suffer more collisions, and come to rest closer to the surface than R_p . As a

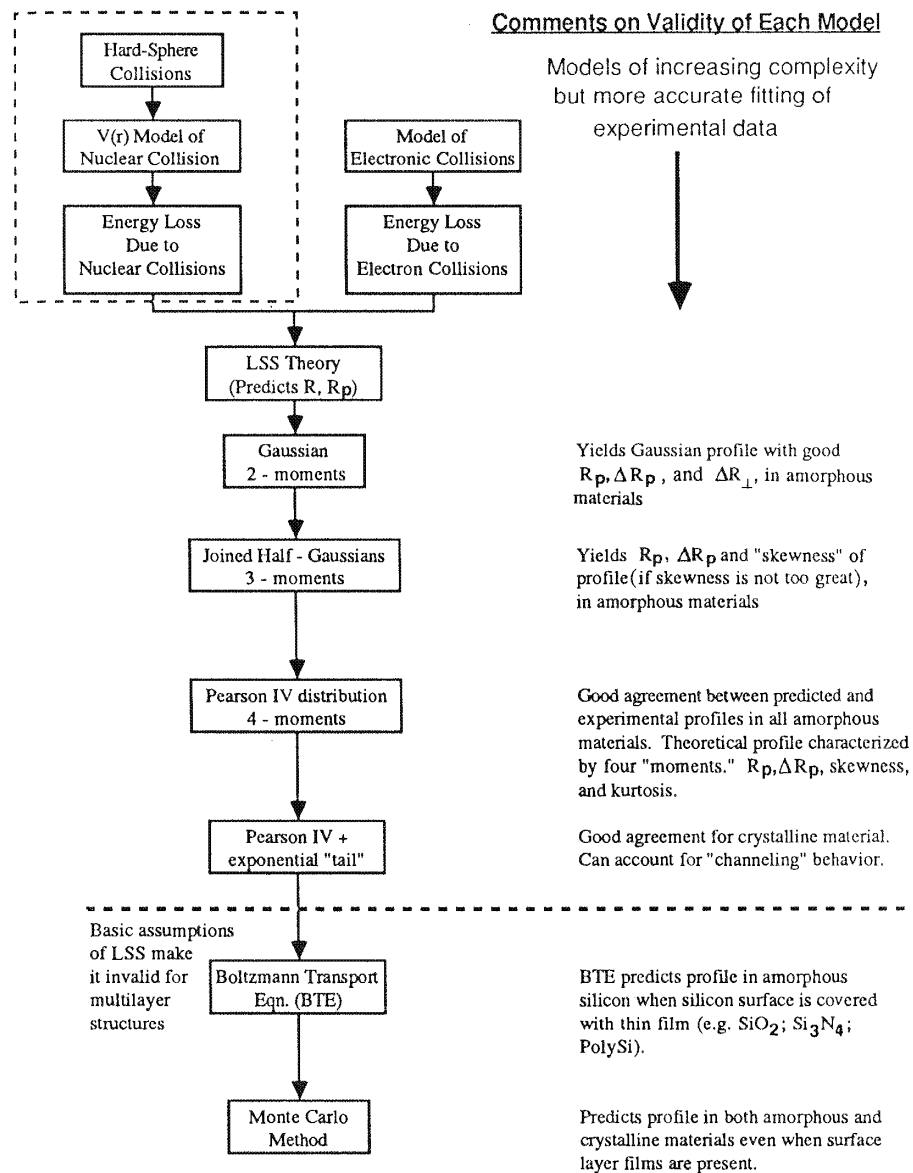


Fig. 10.1 Mathematical models for predicting ion implantation concentration profiles.

result, when large numbers of ions are implanted, R_p corresponds to the depth at which most ions stop, and this is the distance at which the profile has maximum value. The statistical fluctuation along the direction of the projected range is given by the quantity known as the *projected straggle*, ΔR_p (Fig. 10-2b).

The ions are also scattered to some degree along the direction perpendicular to the incident direction, and the statistical fluctuation along this direction is called the *projected lateral straggle*, ΔR_l (Fig. 10-2b). Information about the projected lateral straggle is important because it describes the extent of lateral penetration of ions under the edges of implant masks. Such lateral penetration may represent a limiting dimension in some integrated circuit device structures. In general, values of ΔR_p and ΔR_l are within $\pm 20\%$ of one another. Figure 10-3a shows an opening in a "thick" mask material and resultant ion concentrations in the lateral direction in the target. It is seen that lateral straggle effects cause implanted ions to be distributed under edges of the mask. In Fig. 10-3b contours of equal-ion concentration for 70-keV B atoms implanted into a 1- μm slit are shown.⁶

10.2.2 Theory of Ion Stopping

As an ion moves through a solid target, it transfers energy by collisions with the target nuclei (*nuclear collisions*) and by coulombic interaction with the electrons in the target material. In the latter mechanism, the energy transferred to the electrons can lead to exciting the electrons to higher energy levels (*excitation*), or to the ejection of electrons from their atomic orbits (*ionization*). The energy loss due to such target interactions gradually slows the ion, eventually bringing it to a stop. If the energy of the ion at any point along its trajectory in the target is given by E , the process of *energy loss through nuclear collisions* can be characterized by an *energy loss per unit length due to nuclear stopping*, $S_n(E)$, and *energy loss from interactions with target electrons* by an *energy loss per unit length due to electronic stopping*, $S_e(E)$. The total rate of energy loss $(dE/dx)_{\text{total}}$ is given by the sum of these stopping mechanisms:

$$\left[\frac{dE}{dx} \right]_{\text{total}} = S_n(E) + S_e(E) \quad (10.2)$$

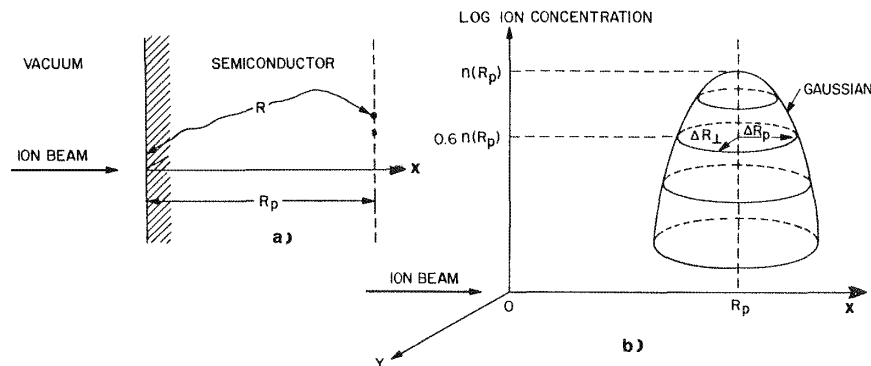


Fig. 10-2 a) Schematic of the ion range, R , and projected range, R_p . b) Two-dimensional distribution of the implanted atoms. From S.M. Sze, *Semiconductor Devices, Physics and Technology*, Copyright © 1985 John Wiley & Sons. Reprinted with permission of John Wiley & Sons.

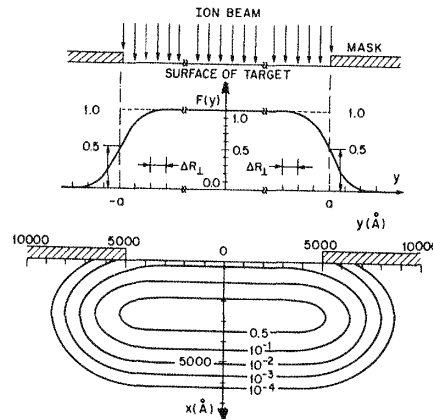


Fig. 10-3 Illustration of lateral profiles. (a) Ion concentration along the lateral direction (y) for a gate mask with $a \gg \Delta R_L$ and infinite extension in the x -direction. (b) Contours of equal-ion concentrations for 70 keV B^+ ($R_p = 2710 \text{ \AA}$, $\Delta R_p = 824 \text{ \AA}$, and $\Delta R_L = 1006 \text{ \AA}$) incident into silicon through a $1 \mu\text{m}$ slit.⁶ Reprinted with permission of the Japanese Journal of Applied Physics.

If the total distance that the ion travels before coming to a complete stop is given by R , then:

$$R = \int_0^E \frac{dR}{(dE/dR)} \quad (10.3)$$

where E_0 is the initial incident ion energy.

The *nuclear stopping process* can be visualized with the aid of the extreme simplification that treats the event as a collision between two hard spheres (Fig. 10-4). A more correct approximation assumes that the scattering is described by a Coulombic force-at-a-distance interaction. In the latter description, an appropriate atomic scattering potential $V(r)$ must be determined. The most successful model for predicting implantation profiles based on the ion stopping approach is the so called *LSS model*, which is discussed in the following section. The LSS model utilizes a modified Thomas-Fermi screened potential for $V(r)$. Calculations based on this model show that nuclear stopping increases linearly in effectiveness at low energies, reaches a maximum at some intermediate energy, and decreases at higher energies (because at high velocity, ions move past target nuclei too quickly to efficiently transfer energy to them). Values of $S_n(E)$ for boron, phosphorus, and arsenic are shown in Fig. 10-5. It is important to note that $S_n(E)$ increases with the mass of the implanted ion, and thus heavy ions such as arsenic will transfer much more of their energy through nuclear collisions than will B atoms.

The *electronic stopping process* can be considered as similar to the stopping of a projectile in a viscous medium, and the stopping magnitude can be approximated to be proportional to the square root of the ion energy:

$$S_e(E) = k_e (E)^{1/2} \quad (10.4)$$

where k_e is a constant that depends weakly on the ion and target atomic masses and numbers. Figure 10-5 also shows $S_e(E)$ for B, P, and As. As can be seen in Fig. 10-5 the crossover energy at which electronic stopping becomes more effective than nuclear stopping is higher for heavier

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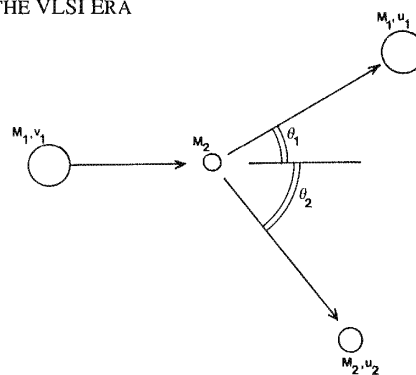


Fig. 10-4 Collision between two particles treated as if they are hard spheres.

ions. For example, for boron $S_e(E)$ is the predominant energy loss mechanism down to ~ 10 keV, while for P and As, the energy loss due to nuclear stopping predominates for energies up to 130 keV and 700 keV, respectively.

10.2.3 Models for Implantation Profiles in Amorphous Solids

The range-energy relation given by Eq. 10-2 was reformulated by Lindhard, Scharff, and Schiott (LSS) for implantation into amorphous material in terms of the reduced parameters ϵ and ρ , as:

$$\frac{d\epsilon}{d\rho} = \left(\frac{d\epsilon}{d\rho}\right)_n + k_\epsilon (\epsilon)^{1/2} \quad (10.5)$$

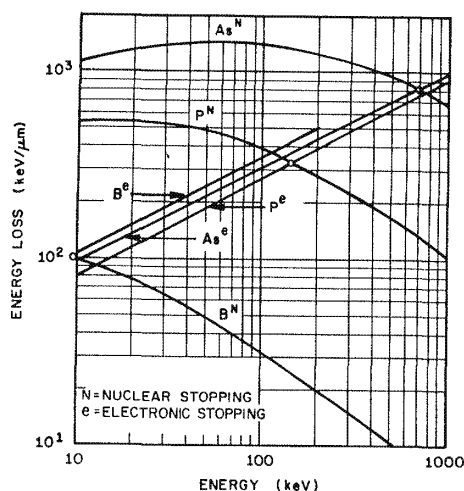


Fig. 10-5 Calculated values of dE/dx for As, P, and B at various energies. The nuclear (N) and electronic (e) components are shown. Note the points (o) at which nuclear and electronic stopping are equal. (After Smith, Ref. 7, redrawn by Seidel in Ref. 83. Copyright 1983, Lucent Technologies, Incorporated, reprinted by permission.)

where ρ and ϵ are dimensionless variables related to the range R , and the incident energy E_0 by:

$$\rho = \frac{(RNM_1M_2/4\pi a^2)}{(M_1 + M_2)} \quad (10.6a)$$

and

$$\epsilon = \frac{E_0 a M_2}{[Z_1 Z_2 q (M_1 + M_2)]} \quad (10.6b)$$

where: M_1 and M_2 are the mass of the incident ions and target atoms, respectively; N is the number of atoms per unit volume; a is the screening length [equal to $0.88a_0/(Z_1^{1/3} + Z_2^{2/3})^{1/2}$, in which a_0 is the Bohr radius and Z_1 and Z_2 are the atomic numbers of the ion and target].

LSS used a modified Thomas-Fermi screened potential to calculate the energy loss due to nuclear stopping, together with the assumption that the energy loss due to electronic stopping is given by Eq. 10-4 (Fig. 10-6). Using this approach, they calculated values of ρ for different values of ϵ . (Note that these calculations are quite complex, but can be found in the classic paper by LSS.³) The value of ρ was then converted to R (using Eq. 10-6a), and finally a value for R_p was obtained from the approximate expression:⁸

$$R_p \approx \frac{R}{1 + \left[\frac{M_2}{3M_1}\right]} \quad (10.7)$$

LSS assumed that the distribution of the implanted ions in amorphous materials could be described by a symmetrical Gaussian curve. If this assumption is valid then the implanted ion concentration, n , as a function of depth, x , can be described by:

$$n(x) = \frac{\phi}{\sqrt{2\pi}\Delta R_p} \exp\left[-\frac{(x - R_p)^2}{2\Delta R_p^2}\right] \quad (10.8)$$

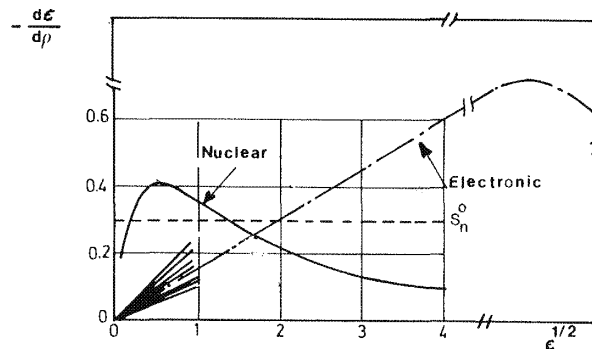


Fig. 10-6 (a) Nuclear stopping power for Thomas-Fermi potential (solid line) and electronic stopping power (dash-dot line) for $k = 0.15$ in terms of the reduced variables ϵ and ρ , based on LSS theory.³

where: ϕ is the dose (in number of implanted ions/cm²), and ΔR_p is the standard deviation of the Gaussian distribution (or *projected straggle* of the distribution in the direction of incidence of the beam). The value of ΔR_p is calculated in terms of R_p and the mass of the implanted ions M_1 and the target atoms M_2 , by the approximate expression:⁸

$$\Delta R_p \cong \frac{2R_p}{3} \left[\frac{\sqrt{M_1 M_2}}{M_1 + M_2} \right] \quad (10.9)$$

The concentration is maximum at R_p , and Eq. 10-8 at $x = R_p$ reduces to:

$$n(x = R_p) = \frac{\phi}{\sqrt{2\pi}\Delta R_p} \cong \frac{0.4R_p}{\Delta R_p} \quad (10.10)$$

The assumption by LSS that the distribution of implanted atoms in amorphous materials is well approximated by a Gaussian curve is not completely correct, but is nevertheless very useful as a first order description. Indeed, the fit to experiment is almost always good for all implantations near the peak. For example, the peak value predicted by Eq. 10-10 is generally within 1% of the measured value (except for very shallow [low energy] implants). On the other hand, significant asymmetries begin to appear in experimental implant profiles in amorphous targets once the concentration levels drop by a factor of 10 below the peak value (and which are not taken into

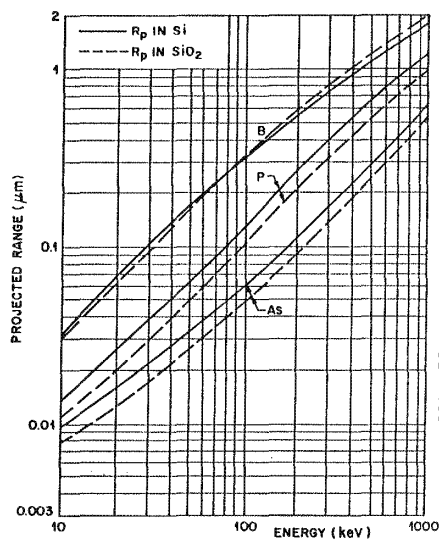


Fig. 10-7 Projected range for B, P, and As in Si and SiO₂ at various energies. The results pertain to amorphous silicon targets and thermal SiO₂ (2.27 g/cm³). After Smith, Ref. 7, redrawn by Seidel in Ref. 83, Copyright, 1983, Lucent Technologies, Incorporated. Reprinted by permission.

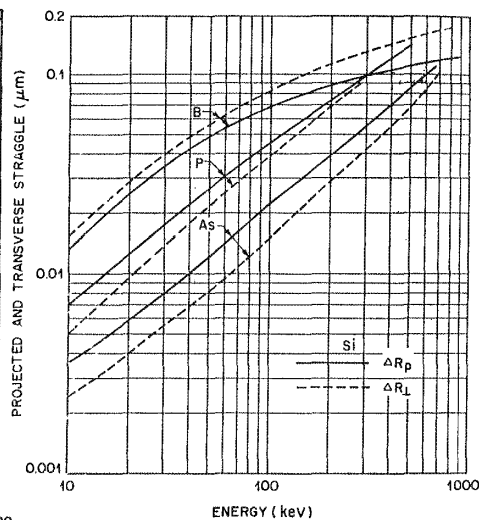


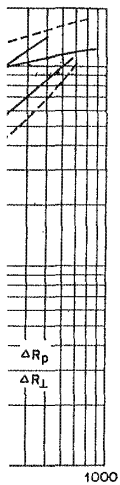
Fig. 10-8 Calculated ion projected straggle ΔR_p , and ion lateral straggle ΔR_L for As, P, and B ions in silicon. After Smith, Ref. 7, redrawn by Seidel in Ref. 83, Copyright, 1983, Lucent Technologies, Incorporated. Reprinted by permission.

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account by a symmetrical Gaussian approximation). Therefore, various distribution curves with a higher number of moments than a Gaussian (which can be described with only two moments, R_p and ΔR_p), have been examined for their ability to fit the experimental implant profiles (Fig. 10-1). In addition, LSS theory and the Gaussian curve fail to account for several effects that occur when implants are made into *single-crystal* material. Thus, modifications (or even other analytical models) must be used to obtain a good fit to data obtained in such situations.

Nevertheless, in practice the Gaussian distribution is still commonly used to provide quick estimates of doping distributions into amorphous and single-crystal targets. The higher moment distributions (or alternate models) are subsequently utilized to fine-tune the dose or energy to obtain better results. Several workers have calculated R_p and ΔR_p values for many of the elements that are commonly implanted into Si and SiO_2 (using LSS theory to perform the calculations). Figure 10-7 is an example of such data for B, P, and As into silicon. Values for projected lateral straggle, ΔR_L , have also been compiled, and are given in Fig. 10-8 (together with ΔR_p).

Example 10-1: A 150 mm wafer is to be implanted with 100 keV boron atoms to a dose of 5×10^{14} ions/cm²: 1) Determine the projected range, projected straggle, and peak concentration using Figs. 10-7 and 10-8. 2) If the implantation time is 1 min, calculate the required ion beam current.

Solution: 1) From Figs. 10-7 and 10-8 it is found that the *projected range* and *projected straggle* are 0.32 μm and 0.07 μm , respectively. The peak concentration, $N(x = R_p)$, can be calculated from Eq. 10-10, or:

$$N(x = R_p) = \frac{0.4 \phi}{\Delta R_p} = \frac{0.4 (5 \times 10^{14} \text{ cm}^{-2})}{(0.07 \times 10^{-4} \text{ cm})} = 2.8 \times 10^{19} \text{ ions/cm}^3$$

2) To find the beam current, first calculate Q , the total number of implanted ions (where $Q = \text{dose} \times \text{wafer area}$):

$$Q = (5 \times 10^{14} \text{ ions/cm}^2) \times [\pi (15/2)^2] = 8.8 \times 10^{16} \text{ ions}$$

Then, the required scanned beam current is determined by dividing the total charge, qQ , by the time of implantation:

$$I = (qQ/t) = [(1.6 \times 10^{-19} \text{ C}) (8.8 \times 10^{16})]/60 \text{ sec} = 0.23 \text{ mA.}$$

10.2.3.1 Higher Moment Distributions for Implant Profiles in Amorphous Material: As noted earlier, even when implanting into amorphous material, the experimental profiles exhibit some asymmetry, or *skewness*. This is not surprising if one considers the forward momentum of the ions. That is, when relatively light atoms make collisions with target atoms (e.g., B in Si), they experience a significant degree of backscattering. Hence more will come to rest at a distance closer to the surface than R_p (causing the concentration near the surface to be higher). On the other hand, heavier atoms will undergo little backscattering, and the concentration on the deep side will be higher. Thus, even if a Gaussian distribution is used to approximate the implantation profile, such non-Gaussian effects on the behavior of devices can be anticipated. That is, when boron is utilized to implant deep p -wells (e.g., in CMOS technology), higher doping close to the surface is observed than is predicted by a Gaussian distribution. On the other hand, the skewness in arsenic implants will produce deeper junctions than predicted when implanting n^+ source/drain (or n^+ emitter regions) with arsenic.

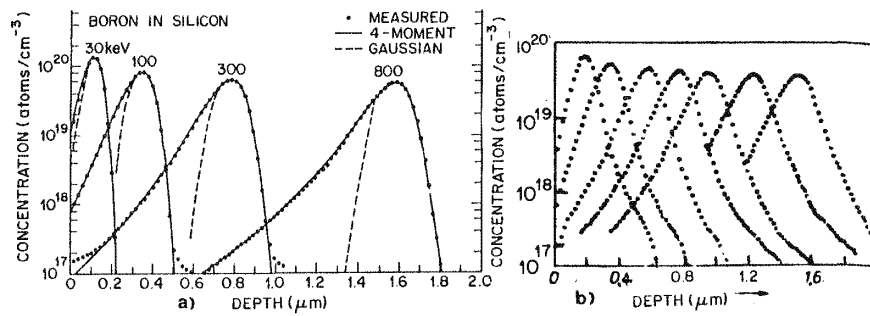


Fig. 10-9 (a) Boron implanted atom distributions, showing 1) measured data points, 2) four-moment (Pearson-IV) curves, and 3) symmetric Gaussian curves. The boron was implanted into *amorphous silicon* without annealing. (b) Depth distributions of boron implanted in *crystalline silicon* in a $\langle 763 \rangle$ direction - a dense crystallographic direction at various energies. *Tails* occur because of channeling effects.⁵ Reprinted with permission of Philips Research Reports.

To theoretically account for the skewness found in measured profiles, probability distributions with higher order moments must be used to approximate impurity distributions. Gibbons and Mylroie⁹ have demonstrated that use of a distribution with a third central moment can closely approximate depth profiles if the asymmetry of the profile is not excessive (i.e., the value of the third central moment is less than ΔR_p). When this approach is taken, the distribution is actually represented by two half-Gaussian profiles, each with their own projected straggle ΔR_{p1} and ΔR_{p2} (Fig. 10-6b), joined together at the depth of their modal range, $R_m = R_p - 0.8(\Delta R_{p1} - \Delta R_{p2})$. The joined half-Gaussian approximation produces a good fit to the profiles of phosphorus and arsenic atoms implanted into Si. The concentration values of such distributions as a function of depth can be calculated from:

$$n(x) = \frac{2\phi}{\sqrt{2\pi}(\Delta R_{p1} + \Delta R_{p2})} \exp\left[-\frac{(x - R_M)^2}{2\Delta R_{p1}^2}\right] \quad x \geq R_M \quad (10.11a)$$

$$n(x) = \frac{2\phi}{\sqrt{2\pi}(\Delta R_{p1} + \Delta R_{p2})} \exp\left[-\frac{(x - R_M)^2}{2\Delta R_{p2}^2}\right] \quad x \leq R_M \quad (10.11b)$$

and the values for ΔR_{p1} and ΔR_{p2} are found in the tabulated data of Gibbons *et al.*²

An approach that represents the implanted profile with a distribution described by *four moments* is more exact than the three-moment approach (and is applicable even when the third central moment is large). In fact, Hofker⁵ demonstrated that excellent agreement with measured B profiles in amorphous Si is obtained (Fig. 10-9), by assuming that the implantation distribution can be described by a *Pearson-IV distribution function*, a type of distribution function which can be specified by four moments. The four moments describe various characteristics of the implant profile curve: 1) μ_1 (mean range); 2) μ_2 (straggle); 3) γ_1

(skewness); and 4) β (*kurtosis* - which characterizes the *tail* aspect of the distribution). It was later shown by Ryssel *et al.*,¹⁰ that equally good agreement is found using a Pearson-IV curve for other implanted species into amorphous targets. The mathematical expressions for the Pearson-IV curve are quite lengthy and fall beyond the scope of this text. However, they can be found in Reference 1.

10.2.4 Implanting Into Single Crystal Materials: Channeling

LSS theory matched with an appropriate distribution curve can accurately predict concentration profiles for implantation into amorphous materials. In practice when fabricating ULSI, however, most implants are made into single-crystal Si. In single-crystal lattices there are some crystal directions (known as *channels*) along which the ions will not encounter any target nuclei, and will instead be *channeled*, or *steered* along such open channels of the lattice. Figure 10-10 illustrates the most likely channeling directions. They are (in order), $\langle 110 \rangle$, $\langle 111 \rangle$, and $\langle 100 \rangle$. These are the directions that exhibit channels of decreasing "openness." As the implanted atoms travel along channels, the slowing down is accomplished mainly by electronic stopping, and the ions can penetrate the lattice several times more deeply than in amorphous targets (Fig. 10-11a). At first, this might appear to offer the advantages of being able to produce deeper implanted junctions and less lattice damage. It turns out, however, that the large sensitivity to incident beam direction, and the unpredictable effects of *dechanneling* (leading to anomalous profile tails), make channeling effects difficult to control. These issues have kept the apparent benefits of channeling from being exploited to produce deep implanted profiles.

Thus, instead of seeking to harness the effect of channeling, techniques have been sought to avoid its occurrence. The most widely adopted procedure to minimize channeling has been to tilt the wafer surface relative to the incident beam direction (most commonly by $\sim 7^\circ$), so that the lattice presents a dense orientation to the incident beam (i.e., the approximate $\langle 763 \rangle$ direction). There are two reasons why this technique *reduces* (but does not eliminate) channeling:

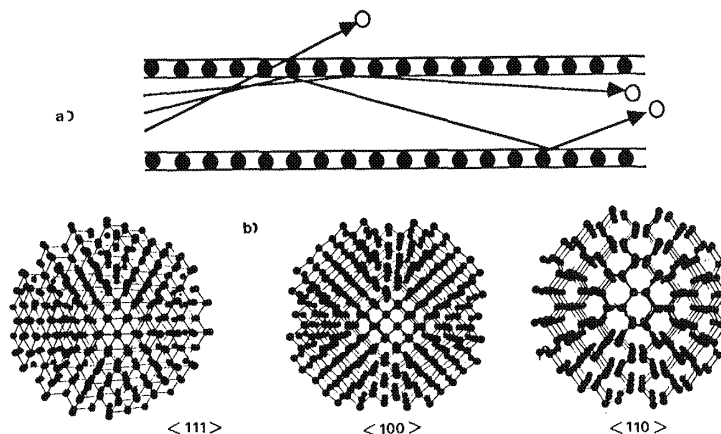


Fig. 10-10 (a) Schematic representation of ion trajectories in an axial channel for various entrance angles. (b) Ball model showing relative degree of "openness" of the diamond (Si) lattice when traversing in $\langle 111 \rangle$, $\langle 100 \rangle$, and $\langle 110 \rangle$ directions.

1. Even when atoms enter the lattice in an apparently random, "dense-appearing" direction, they can be diverted into one of the open channels after entering the lattice (Fig. 10-11b). This effect leads to the *tails* that are observed in implanted profiles into single-crystal lattices. Figure 10-9b shows the depth profiles of boron implanted into crystalline Si in a $\langle 763 \rangle$ direction. Compared to Fig. 10-9a, it can be seen that tails in the profile exist. The combination of "random" and "channeled" atoms can be used to construct a highly accurate description of the net implant profile, as illustrated in Fig. 10-12.

2. If the 7° tilt is performed such that the Si atoms are still inadvertently aligned in a highly symmetric array of planes, the phenomenon of *planar channeling* can still produce channeling effects (Fig. 10-13). Turner *et al.*¹³ reported that in order to insure that both planar and axial channeling effects are avoided, wafers must also be oriented with an appropriate azimuthal (or *twist*) direction, in addition to a proper tilt angle.

Recommended optimum twist angles for various implantation species, energy, and orientation are shown in Fig. 10-13. It should be noted that control of the twist angle was not possible with many of the gravity-fed wafer handling systems used on older medium-current implanters. However, most implanter suppliers now provide end-stations that make provision for controlling twist angle.

In addition to tilting and twisting wafers, other methods investigated to further reduce

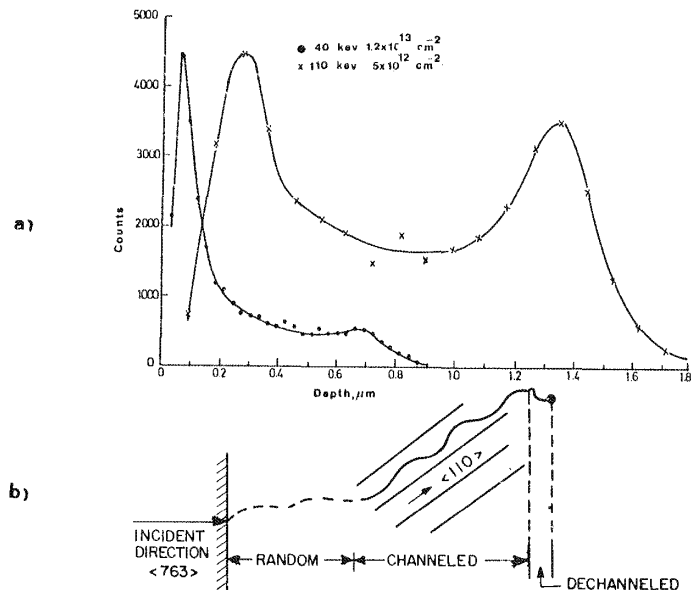


Fig. 10-11 (a) Variation of P32-concentration profiles with ion energy for implantation along $\langle 110 \rangle$ axis, plotted on a linear scale.¹¹ Reprinted with permission of Canadian Journal of Physics. (b) Schematic diagram of an ion path in a single crystal for an ion incident in a "dense" $\langle 763 \rangle$ direction. The path shown has non-channeled and channeled behavior.⁶³ Copyright, 1983, Lucent Technologies, Incorporated, reprinted by permission.

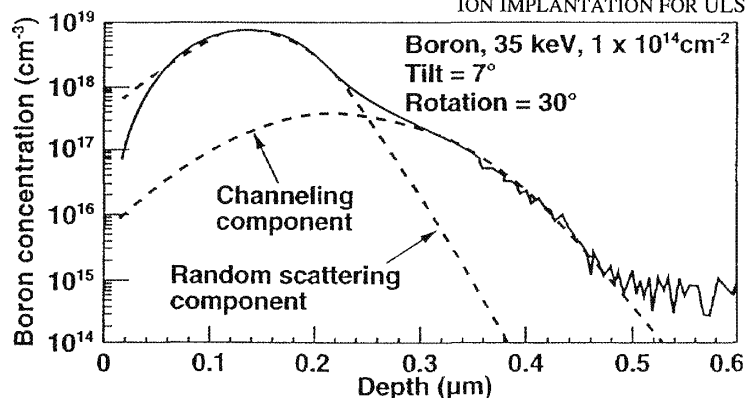


Fig. 10-12 Illustration of a one-dimensional dual Pearson model. The dotted line is the model prediction, and the solid line is the experimental profile measured by secondary ion mass spectroscopy.¹²

channeling effects include: a) pre-amorphizing the lattice by a prior implantation (e.g., with Si or Ge);^{14,15} b) implanting through a surface oxide (to randomize the directions of the ions as they enter the lattice);^{14,15,16} and c) using heavy ions for the implantation (e.g., BF_2 rather than B). These and other issues associated with channeling are discussed in detail by Simonton.¹⁷

10.2.5 Calculating Implantation Profiles: Boltzmann Transport Equation and Monte Carlo Approaches

When fabricating integrated circuits, ion implantation is frequently performed through a thin surface layer (e.g., SiO_2 , Si_3N_4 , or even a composite layer). As discussed in a later section, if the stopping powers of the various layers are not too different, simple approximations can be used to fit actual profiles fairly well. More accurate predictions of profiles into multilayered materials, however, require either a numerical solution of the Boltzmann transport equation (BTE)^{18,19} or a Monte Carlo simulation.^{20,21} The assumption used by the LSS theory that the target material is homogeneous and isotropic makes the LSS model invalid for predicting implantation ranges in multilayer structures. In both the BTE and Monte Carlo methods, the predicted distribution is calculated directly (rather than inferred from a range value and an assumed distribution curve).

Accurate and "computationally efficient" as-implanted profiles are needed as the inputs to the process simulators that calculate dopant diffusion (such as SUPREM and FLOOPS). Such as-implanted doping profiles are available from a large body of experimental data on dopant range profiles that has been organized into multi-parameter fits for "random" (or "amorphous material") and "channeled" (or crystalline material) profiles. The two types of profiles are each fit to a Pearson-IV distribution with the ratio of the random to channeled portions related to the damage and accumulated dose. In recent implementations of this approach, the Pearson-IV distributions have been replaced by the more general Legendre polynomials.^{12,22,82}

10.2.5.1 Monte Carlo Calculations: In the Monte Carlo approach, ion implantation is simulated by following the history of an energetic ion through successive collisions with target atoms using the binary collision assumption. The calculation of each trajectory begins with a given energy, position, and direction. A large number of ion trajectories are calculated ($>10^3$), and the

depth at which each ion stops is determined. The predicted profile is generated by plotting histograms of the number of ions stopped within each depth interval. Monte Carlo simulations can be performed for either amorphous or crystalline targets. In the amorphous material simulation, the position of the target atoms follows a Poisson distribution, while in crystalline target simulation the atom positions are specified to correspond to the positions that they would assume on a lattice.

A widely used, PC-based Monte Carlo range and damage simulation program is named TRIM (for Transport of Ions in Matter).²³ It assumes that the target material is amorphous (i.e., no channeling effects occur), and consequently provides a very useful first-approximation to the atom range and damage distributions in multi-element and multi-layer materials.²⁴ A more advanced Monte Carlo code has been developed for Si-like crystalline targets (UT-MARLOWE). It runs on Unix-based workstations and provides highly accurate atom range and damage distributions (including the effects of damage accumulation on channeled profiles).^{84,85}

10.3 ION IMPLANTATION DAMAGE ACCUMULATION AND ANNEALING IN SILICON

As discussed earlier, ion implantation has many advantages for ULSI processing, the most important being the ability to control (to a high degree of precision) the number and depth of impurity atoms introduced into a substrate. The price for such benefits is high, however, as implantation cannot be achieved without damage to the substrate material. That is, high-energy ions collide with substrate atoms and displace them from their lattice sites in large numbers. Furthermore, only a small percentage of the as-implanted atoms end up on electrically active lattice sites. In order to successfully fabricate devices, the damaged substrate regions must be

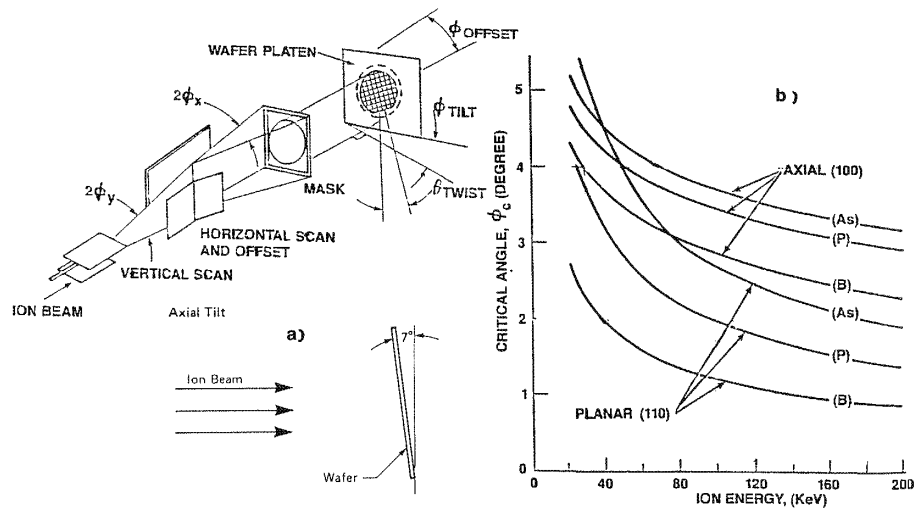


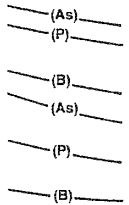
Fig. 10-13 (a) Channeling avoidance by using axial tilt and azimuthal twist. (b) Calculated critical angles vs. ion energy for channeling along the axial Si $\langle 100 \rangle$ direction and planar $\langle 110 \rangle$ direction for B^+ , P^+ , and As^+ ions.¹³ Reprinted with permission of Solid State Technology, published by PennWell.

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must be restored to their pre-implanted structure, and the implanted species must be electrically activated. Described in this section are: a) the aspects of implantation damage; b) the mechanisms of damage annealing; and c) the electrical activation of implanted dopants. Figure 10-14 illustrates the subjects that will be covered. At the conclusion of the section it will be noted that as devices are designed with very shallow junctions (e.g., ≤ 250 nm deep), the remaining residual implantation damage (even after the annealing process) represents a mechanism that degrades device operation. An example is the excess reverse-bias leakage current observed when such shallow junctions are fabricated.

10.3.1 Implantation Damage in Silicon

When energetic ions strike a silicon substrate they lose their energy in a series of nuclear and electronic collisions, and thus rapidly come to rest some hundreds of atom layers below the surface. Only the nuclear collisions result in *displaced silicon atoms* (also referred to as *damage* or *disorder*). An individual nuclear collision can result in different types of displacement events, depending upon the magnitude of the energy transferred.

If the energy transferred to a silicon atom (ΔE_n) is less than the energy required to displace it from its lattice site, E_{di} , no displacement event results. If $2E_{di} \geq \Delta E_n \geq E_{di}$, a single displacement and simple isolated point defects are created. If $\Delta E_n \geq 2E_{di}$, point defects and *secondary displacements* (i.e., recoiled lattice atoms with enough energy to generate additional lattice disorder) are produced. Finally, if $\Delta E_n \gg 2E_{di}$, multiple secondary displacements and defect clusters are created. (Note, $E_{di}[\text{Si}] \sim 15$ eV.)

Because of their extremely small size, the exact nature of isolated defects and defect complexes from ion implantation are hard to characterize. However, each displacement of a lattice atom (whether by a primary beam ion or an energetic recoil lattice atom), produces a *Frenkel defect* (see Chap. 2). In addition, it is widely agreed that the defects include: a) vacancies [V]; b) di-vacancies [V^2] (i.e., two vacancies bound together); c) higher order vacancies and (vacancy-impurity complexes); and d) interstitials [I]. The ions create zones of gross disorder populated by such defects in regions where they deposit their kinetic energy (Fig. 10-15). These zones are vacancy-rich at the center, and are surrounded by [I], since each displaced Si atom moves into the lattice with velocity components perpendicular to the ion track.

The lattice in these disordered regions exhibits several different damage configurations:

1. *Isolated point defects or point defect clusters in essentially crystalline silicon* (i.e., the type of damage that results from implanting light ions, or when $\Delta E_n \approx 2E_{di}$).
2. *Local zones of completely amorphous material* in an otherwise crystalline layer (i.e., an *amorphous region* is defined as a region in which the displaced atoms per unit volume approach the atomic density of the semiconductor). Local zones of amorphous damage are associated with low-dose implants of heavy ions (i.e., $\Delta E_n \gg E_{di}$).
3. *Continuous amorphous layers* which form as the damage from the ions accumulates. That is, as the dose of ions (typically heavy ions) increases, the locally amorphous regions eventually overlap, and a continuous amorphous layer is formed.

In our discussion Type-1 and Type-2 damage will be grouped into the category of *primary crystalline-defect damage*. Type-3 damage will be referred to as *amorphous layer damage*. The basis for this grouping (as shall be seen in the sections that discuss damage annealing), is that the annealing strategy for Type-1 and Type-2 damage are the same, but a different annealing procedure is employed for Type-3 damage.

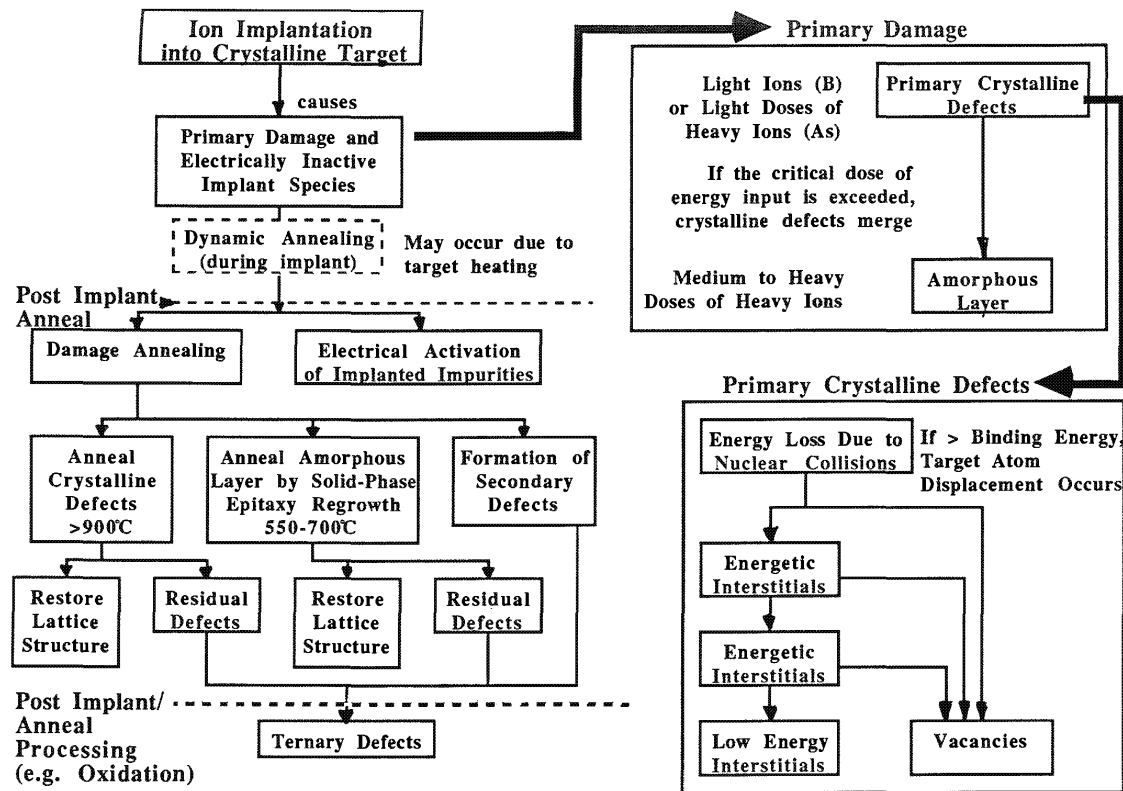


Fig. 10-14 Ion implantation damage and annealing.

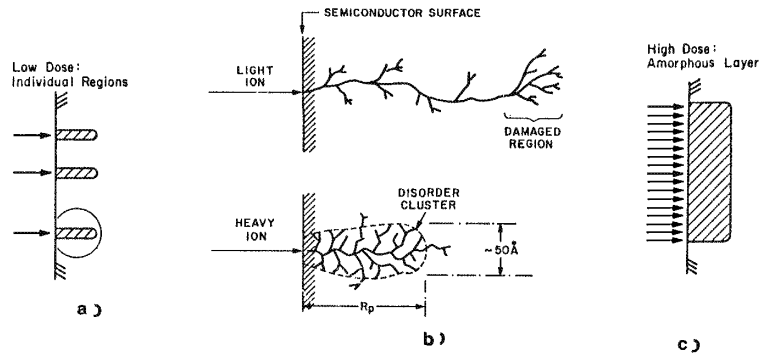


Fig. 10-15 Schematic representation of the disorder produced by ion implantation. (a) Low dose light ions - individual regions with degree of disorder increasing as ions penetrate deeper into substrate. (b) Low dose heavy ions - individual regions of more uniform disorder along entire ion trajectory. (c) Heavy doses - formation of an amorphous layer.

Regardless of the form of the damage configuration, the number of displaced atoms after implant is almost always larger than the number of implanted atoms. These displaced atoms reduce the mobility in the damaged regions and produce defect levels in the band gap of the material (i.e., deep-level traps, for both electrons and holes) which have a strong tendency to capture free carriers from the conduction and valence bands. Due to the relatively large number of displaced atoms (and the fact that few as-implanted impurities occupy substitutional sites), non-annealed implanted regions typically exhibit high resistivity.

10.3.2 Primary Crystalline Defect Damage

Primary crystalline defect damage is observed after implanting a Si crystal (28 atomic mass units [28 amu]) with relatively light ions (e.g., B [11 amu]), or with light doses of heavier ions (e.g., P [31 amu], As [75 amu], and Ar [40 amu]). As noted in the previous section, the damage configurations from light ions are in fact quite different than those from heavy ion implantation. The reason for the difference is discussed below.

As shown in Fig. 10-5, at the initial impact energies most of the energy loss for *light ions* (in this example, boron) is due to electronic collisions (which do not produce displacement damage). However, as B ions penetrate deeper into the lattice, they lose energy. Eventually, the cross-over energy is reached, below which nuclear stopping predominates ($\sim 10 \text{ keV}$ for B). As shown in Fig. 10-15, *most lattice damage occurs in the part of the light ion trajectory beyond that point*.

An estimate of the damage can be calculated by considering the case of an 80-keV boron ion. Its projected range is $\sim 250 \text{ nm}$ (Fig. 10-7), and its initial *nuclear energy loss* is $\sim 35 \text{ eV/nm}$ (Fig. 10-5). The boron ion will thus lose $\sim 8.75 \text{ eV}$ from nuclear collisions for each lattice plane that it passes (as the lattice spacing in Si is $\sim 0.25 \text{ nm}$). Since 8.75 eV is less than $E_{di} [\text{Si}]$, the B atom (upon initially entering the Si), does not transfer enough energy per nuclear collision to displace silicon atoms from their lattice sites. When the ion energy has decreased, however, to 40 keV (at a depth of $\sim 130 \text{ nm}$ in the lattice), the energy loss due to nuclear collisions rises to $\sim 15 \text{ eV per}$

lattice plane (i.e., 60 eV/nm), which is sufficient to displace Si lattice atoms. (Note that although electronic stopping is still predominant, nuclear stopping between 10–40 keV can still displace Si atoms.) Assuming that one Si atom is displaced per lattice plane for the remainder of the ion trajectory, 480 lattice atoms are displaced (i.e., 120 nm/0.25 nm) by the time the boron atom comes to complete rest. If each displaced atom is moved roughly 2.5 nm by such collisions, the damage volume is found from $V_{\text{dam}} \cong \pi (2.5\text{ nm})^2 (120\text{ nm}) = 2.4 \times 10^{-18}\text{ cm}^3$. The damage density is $480/V_{\text{dam}} \cong 2 \times 10^{20}\text{ cm}^{-3}$, which amounts to only ~0.2% of the atoms. This calculation implies that very large doses of light ions are required to produce an amorphous layer, and for the most part each ion produces a trail of well-separated primary recoiled Si atoms in the wake of the implanted ion. Furthermore, displaced atoms will be separated by short distances from the vacancies they leave, because the energies of their recoils are low. This suggests that only a relatively small input of energy to the lattice could cause such separated pairs to rejoin. In fact, as will be explained in the following section on annealing, a large fraction of the disorder produced during boron implantations is *dynamically annealed during the implantation*, and therefore at room temperatures even high-dose boron implantations may not produce an amorphous layer. The damage from boron implantations is thus characterized by *primary crystalline defects*. Damage density is distributed versus depth as shown in Fig. 10-16a, which shows a sharp buried peak concentration and qualitatively fits the description of the damage-creation process.

When *heavy ions* are implanted, the energy loss is predominantly due to nuclear collisions over the entire range of energies experienced by the decelerating heavy ions (Figs. 10-5 and 10-15). Thus, substantial damage is expected. Examine the case of 80-keV arsenic atoms, which will have a projected range of ~50 nm. The average energy loss due to nuclear collisions will be ~1200 eV/nm over the entire range. As a result, the As atoms lose ~300 eV for each Si atomic plane that they pass. Most of this energy is transferred to a single lattice atom. The recipient Si atom, however, will subsequently produce ~20 displaced lattice atoms. The total number of displaced atoms is thus 4000. Again, assuming an average distance moved for each displaced atom of ~2.5 nm, the damage volume is $V_{\text{dam}} \cong \pi (2.5\text{ nm})^2 (50\text{ nm}) = 0.8 \times 10^{-18}\text{ cm}^3$. The damage density is then $4000/V_{\text{dam}} \cong 5 \times 10^{21}\text{ cm}^{-3}$, or ~10% of the number of atoms in the lattice within the damage volume. Since a single ion is capable of producing such heavy damage, it is reasonable to expect that some local regions of a silicon substrate (which when subjected to even light doses of heavy-ion bombardment) will suffer enough damage to become amorphous. Some damage density distributions due to heavy-ion (e.g., As) implants are shown in Fig. 10-16b. They exhibit a *broad* buried peak that is a replica of recoiled range distribution.

10.3.3 Amorphous Layer Damage

Simple qualitative concepts illustrate how continued bombardment by heavy ions will lead to the formation of continuous amorphous layers. That is, heavy-ion damage accumulates with ion dose through an increase in the density of localized amorphous regions. Eventually these regions overlap, and a continuous amorphous layer is the result. The evolution of a continuous amorphous layer from the accumulation and overlap of damage formed by individual atoms has been observed (Fig. 10-17) using Rutherford backscattering spectroscopy in a channeling mode. In Fig. 10-17a it can be seen that damage produced by 1.7 MeV Ar^+ ions in Si builds up to an initial damage distribution with a peak at a depth of ~1.3 μm . At that depth, individual amorphous zones are likely to be created by each ion (Fig. 10-17b). Closer to the surface the damage consists predominantly of isolated defect clusters (akin to the damage caused by light

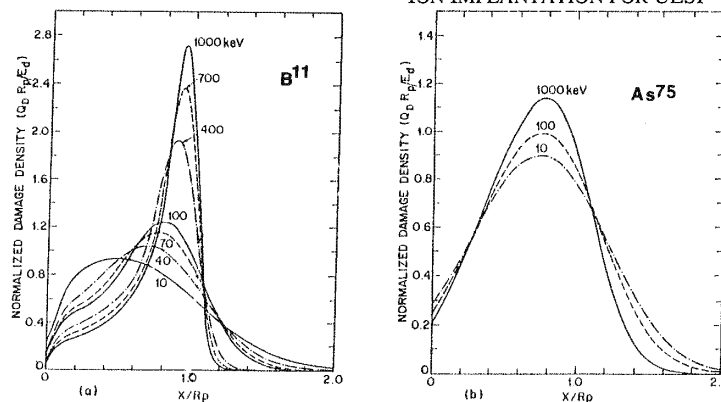


Fig. 10-16 Calculated damage density profiles of (a) boron, and (b) arsenic.²⁵ Reprinted with permission of Plenum Publishing Company.

ions.) As the dose is increased, both types of damage increase, and finally a 1.5 μm -thick, (almost continuous, as in the example of Fig. 10-17a) amorphous layer extends to the surface. This also illustrates another aspect of the formation of amorphous layers. That is, amorphization begins at the depth of the maximum nuclear collision energy deposition, at slightly less than the projected range, and spreads towards the surface (as well as towards deeper positions in the target). In addition, the interface with the single-crystal region below is not a well-defined plane, due to the statistical nature of the penetration. Beyond the interface, primary crystalline damage as well as a considerable concentration of Si interstitials (which had diffused out of the damage clusters during implantation) is expected.

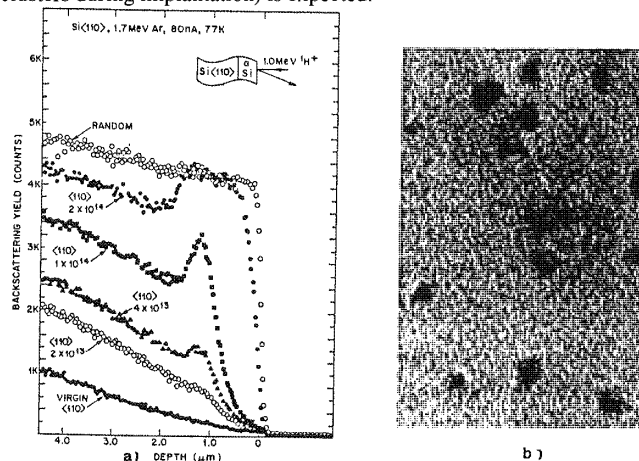


Fig. 10-17 (a) RBS channeling spectra of damage accumulation in Si at liquid nitrogen temperature following bombardment with 1.7 MeV Ar^+ ions.²⁶ By permission of the Harvard University Archives. (b) Bright-field electron micrographs of amorphous regions in Si produced by bombarding to doses of $3 \times 10^{11} \text{ cm}^{-2}$ with 10 keV bismuth ions.²⁷ Courtesy of the Institute of Physics Conference Series.

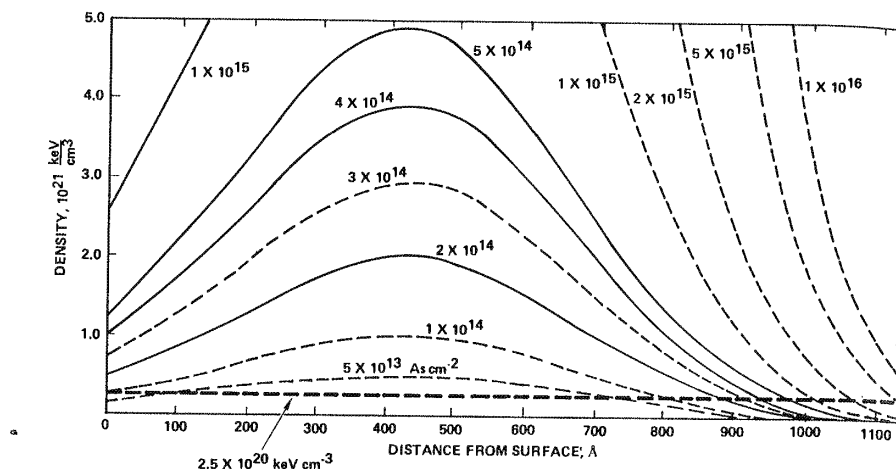


Fig. 10-18 Damage density distribution for 100-keV As implantations for doses of 5×10^{13} – 1×10^{16} As cm^{-2} calculated from Brice's²⁵ curves.²⁸ Reprinted by permission of American Physical Society.

The minimum (or *threshold*) dose required to convert a crystalline material to an amorphous layer can be arrived at from a number of different viewpoints. First, it is certain that when the number of stably displaced Si atoms reaches the number of Si atoms/unit volume (e.g., $5 \times 10^{22} \text{ cm}^{-3}$), the material has become "amorphous." When the damage density reaches this value, an amorphous condition is reached. Another view holds that there is a critical energy density that must be placed into the crystal to make it amorphous.²⁹ This critical energy density E_c is given by:

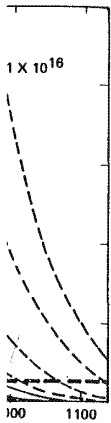
$$E_c \cong f (10^{21} \text{ keV/cm}^3) \quad (10.12)$$

and the pre-factor f is 0.1–0.5 for Si. Based on this model, Brice published tables that predict the extent of the amorphous layer formation for different doses (and constant implant energy). Prussin *et al.*,²⁸ plotted the data from these tables for As implanted into Si (Fig. 10-18). A simple estimate can also be obtained by assuming that if enough energy is applied to the crystal to cause melting (for Si, 10^{21} keV/cm^3); this would also produce an amorphous layer. For 100-keV As ions, the dose D_{crit} calculated from this approach (where E_0 is the beam energy in keV, and R_p in cm), is:

$$D_{\text{crit}} = [(10^{21} \text{ keV/cm}^3) R_p] / E_0 = 6 \times 10^{13} \text{ ions/cm}^2 \quad (10.13)$$

From the discussion on minimum implant dose for creating an amorphous layer, three more important aspects of amorphous layer structure can be inferred:

1. From Brice's model (Fig. 10-18), it can be seen that some implant doses will cause an amorphous layer to form below the surface of the Si, but that near the surface not enough energy has been transferred to the lattice to cause the material to become amorphous (e.g., in the case of As at 100 keV, for doses less than $1 \times 10^{14} \text{ cm}^{-2}$, the energy density at the surface drops below the threshold required to create an amorphous layer). Thus the amorphous region does not extend all the way to the surface, but is a *buried amorphous layer*. Such buried amorphous layers have been found to exhibit profoundly different annealing characteristics than those that extend all the way to the surface.



$10^{16} \text{ As cm}^{-3}$

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2. In the crystalline layer just below the amorphous layer, the silicon was the recipient of impurity atoms, albeit in lower quantities than necessary to cause an amorphous region. Yet, heavy primary-crystalline-defect damage from the implanted ions exists in this zone, as well as implanted impurity atoms that must be electrically activated in order to achieve the full electrical activation of the dose. These cannot be ignored when considering an annealing strategy for amorphous layers.

3. Prussin *et al.*,²⁸ have shown that the critical energy, E_c , required to create an amorphous layer depends on the implanted species, and is $2.5 \times 10^{20} \text{ keV/cm}^3$, $1.0 \times 10^{21} \text{ keV/cm}^3$, and $5.0 \times 10^{21} \text{ keV/cm}^3$, for As, P, and B, respectively.

The temperature of the substrate during implantation also impacts amorphous layer formation. Figure 10-19 shows a plot of the critical dose versus reciprocal temperature for various ions.²⁸ It can be seen that for light ions such as B^{11} , a 50°C rise above room temperature prevents the formation of an amorphous layer at any dose. This is due to the fact that B generates only a few stably displaced atoms during implantation, and a small increase in T above room temperature allows such closely spaced vacancy-interstitial pairs (Frenkel defects) to recombine.

10.3.4 Electrical Activation and Implantation Damage Annealing

In this section the methods that can be used in attempts to restore the silicon to its pre-implanted structure, and to electrically activate the implanted impurity atoms are considered. The subjects will be covered in the following order: a) electrical activation of implanted impurities; b) annealing primary crystalline defect damage; c) annealing of amorphous layers; d) dynamic annealing effects; and e) diffusion of implanted impurities.

10.3.4.1 Electrical Activation of Implanted Impurities: Since most as-implanted impurities do not occupy substitutional sites, a subsequent thermal step is employed to bring about electrical activation. The degree to which the thermal procedure is effective in electrically activating impurities is commonly determined by Hall effect measurements, but can also be checked more simply by measuring the sheet resistance, R_s .³⁰ To a first approximation, R_s is inversely proportional to the mobility μ and the implanted dose ϕ (cm^{-2}):

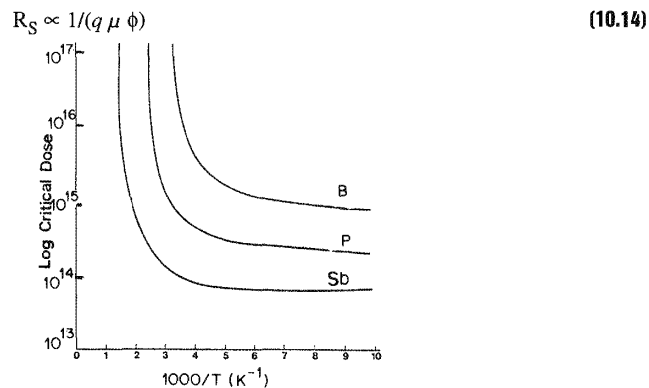


Fig. 10-19 Theoretical relationship between amorphous threshold and temperature for B^+ , P^+ , and Sb^+ into Si.²⁹ Reprinted with permission of Gordon and Breach Publishing Company.