Lecture 3

Diffusion

Reading:

Chapter 3

Impurity Diffusion:

Pfann patented the idea of using diffusions in Si and Ge in 1952. Diffusions are most commonly used for:

      1.) Annealing of ion implanted regions

      2.) Bases, emitters, sometimes collectors and resistors in bipolar technology

      3.) Form source and drain regions and dope polysilicon gate/interconnect lines in MOS technology.

When to use it and when not to use it:

      1.) Use when damage from Ion Implantation leads to unacceptable decreases in Minority carrier lifetime, electrical junctions need to be very deep, or a cheap easy solution is needed.

      2.) Do not use it for ultra-shallow junctions, majority carrier devices (use ion implantation instead) or total impurity "dose" is critical (ex. MOSFET channel)

Diffusions sources include:

      1.) Chemical source in a vapor at high temperature.

      2.) Doped oxide source (either deposited at high temperature or as a "Spin on polymer).

      3.) Diffusion/annealing from an Ion implanted source.

Impurity Diffusion:
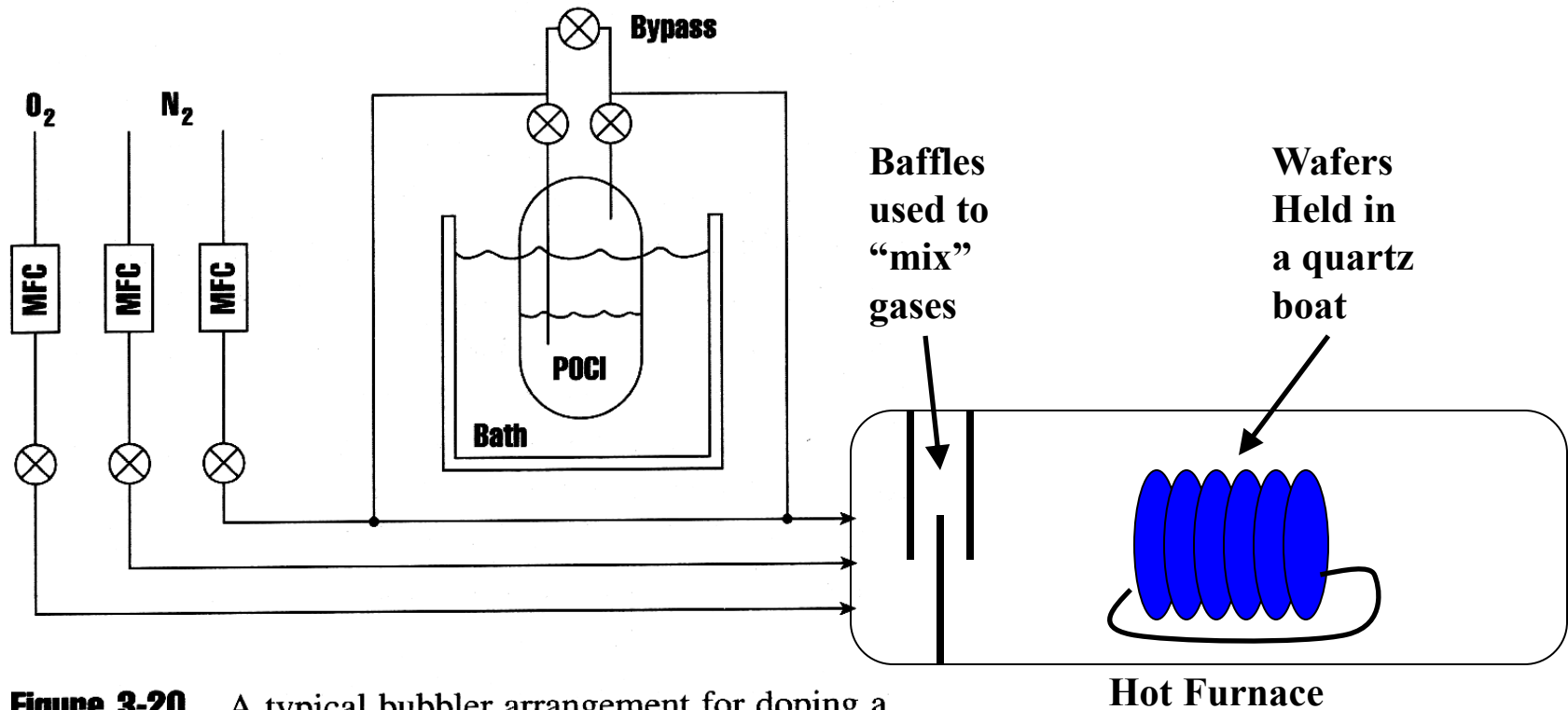## Traditional Tube Furnace

Figure 3-20 A typical bubbler arrangement for doping a silicon wafer using a POCl source. The gas flow is set using mass flow controllers (MFC).

Impurity Diffusion:

Fick's first law states that "impurities" flow (with flux J) toward a decrease in concentration,

$$J = -D \frac{\partial C(x,t)}{\partial x} \qquad \textbf{(1)}$$

The diffusion coefficient, D, also called diffusivity, or diffusion constant, characterizes a particular impurity's resistance to flow when exposed to an impurity gradient.
We do not measure impurity gradients or impurity fluxes. These quantities are difficult to obtain.

Thus, using the law of conservation of matter,

$$\frac{\partial C(x,t)}{\partial t} = -\frac{\partial J}{\partial x} \qquad \textbf{(2)}$$

This second law simply states that the total change in flux leaving a volume equals the time rate of change in the concentration in the volume.

Impurity Diffusion:

Plugging (1) into (2), one can rewrite Fick's first law as Fick's second law,

$$\frac{\partial C(x,t)}{\partial t} = \frac{\partial}{\partial x}\left(D \frac{\partial C(x,t)}{\partial x} \right) \qquad \textbf{(3)}$$

In certain special cases, D is independent of x,

$$\frac{\partial C(x,t)}{\partial t} = D \frac{\partial^2 C(x,t)}{\partial x^2} \qquad \textbf{(4)}$$

We will examine various solutions of this differential equation later.

More generally in 3D:

$$\frac{\partial C}{\partial t} = \nabla \bullet (D \nabla C) \qquad \textbf{(5)}$$

Note that generally, D=f(T , x , and even C).

Impurity Diffusion:
Diffusion Coefficient

What distinguishes one impurity from another is its diffusivity.
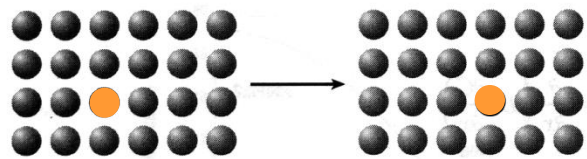
Consider the general case where an atom can exist as both a substitutional or interstitial impurity. We can define a few terms:

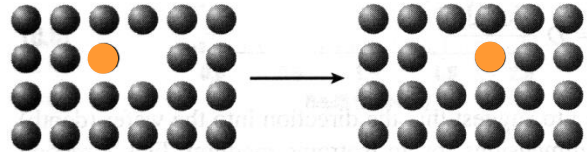$[N_S]$ = Solubility of the impurity in a substitutional site

$[N_I]$ = Solubility of the impurity in an interstitial site

γ_s = Substitutional jump frequency (~10^{13} Hz, depends on Temperature, other factors)

γ_i = Interstitial jump frequency

Impurity Diffusion:
Diffusion Coefficient

Figure 3-3 Diffusion of an impurity atom by direct exchange (b) and by vacancy exchange (a). The latter is much more likely due to the lower energy required.

$$\frac{[N_s]}{[N_s]+[N_i]} \equiv \textit{Fraction of time the impurity spends at the Substitutional Lattice sites}$$

$$\frac{[N_i]}{[N_s]+[N_i]} \equiv \textit{Fraction of time the impurity spends at the Interstitial Lattice sites}$$

then the effective jump frequency can be defined as,

$$\gamma_{effective} = \gamma_s \frac{[N_s]}{[N_s]+[N_i]} + \gamma_I \frac{[N_I]}{[N_s]+[N_i]}$$

Impurity Diffusion:
Diffusion Coefficient

For an interstitial, no defect must be created before the impurity can diffuse. Thus, the diffusivity is,

$$D_{Interstitial} \propto \gamma_{effective} d^2 e^{\left(-E_{motion}/kT\right)}, where\ E_{motion} \sim 0.1 - 1.2\ eV\ for\ Si$$

where d is the distance for a jump.

For a substitutional impurity to move, it must first "create" a vacancy-interstitial pair. Thus, often its motion is limited by the energy required to create the defect

$$D_{substitutional} \propto \gamma_{effective} d^2 e^{\left(-\left(E_{defect\ creation} + E_{motion}\right)/kT\right)}, where\ E_{defect\ creation} \sim 4 - 5\ eV\ for\ Si$$

Generally,

$$D = D_o e^{\frac{-E_a}{kt}}$$

Note: D_o is assumed constant but in fact has a slight dependence on temperature through the $\gamma_{effective}$ term.

Impurity Diffusion:
Surface Diffusion Coefficient (Controls Epitaxy)

Generally,

$$D = D_o e^{\frac{-E_a}{kt}}$$

Exponential Dependence Surface Barriers

$$\text{Hopping Rate} = \gamma e^{-\phi/kT}$$

Vibration Frequency ~10^{13} Hz (slightly T dependent)

Exponential Dependence on Temperature

$$\text{Surface Diffusivity} = \left[d^2 \left(\frac{\gamma}{4} \right) \right] e^{-\phi/kT}$$

D_o

Strong Bonds in Wide Bandgap Semiconductors Cause Desorption and Diffusion to be Competitive
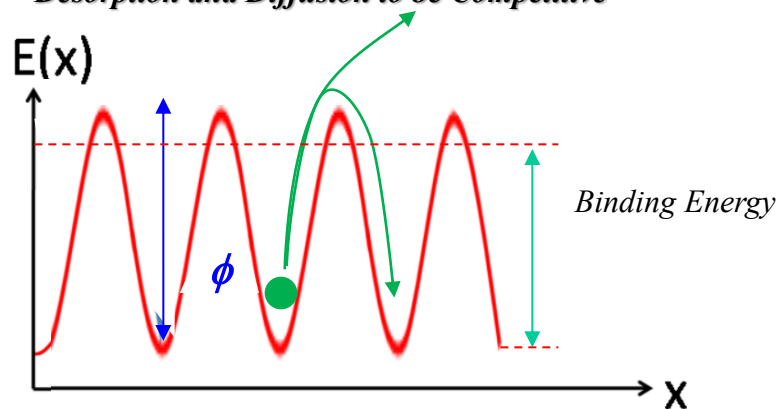
Weaker (Metal-like) Bonds Increase Diffusion Even at Low Temperatures

Note: D_o is assumed constant but in fact has a slight dependence on temperature through the hopping frequency, γ, term.

Impurity Diffusion:
Bulk Diffusion Mechanisms
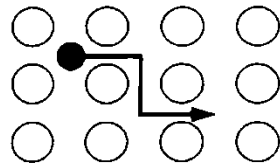
Interstitial mechanism
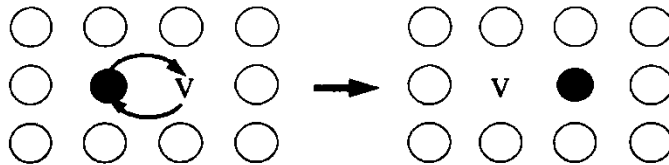
Vacancy mechanism
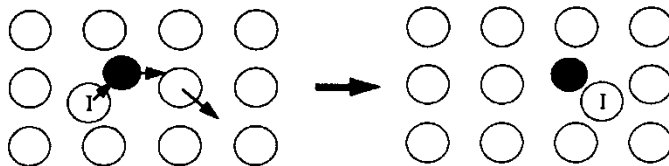
Interstitialcy mechanism
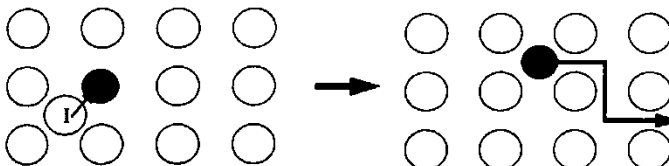
Kick-out mechanism
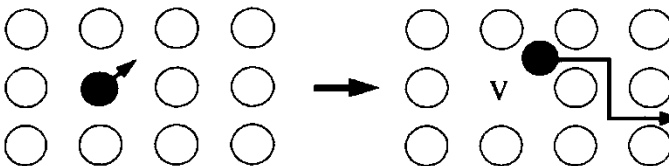
Dissociative mechanism

The diffusivity is dependant on the point defect reactions that take place. Several mechanisms exist: Interstitial, vacancy, interstitialcy, and dissociati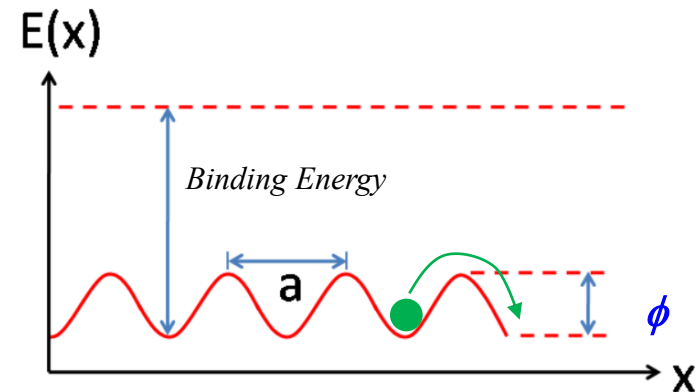ve mechanisms. Note: the kickout mechanism is a subset of the full interstitialcy mechanism but does not require the presence of self-interstitials.

Figure 5.1 Schematic representation of different diffusion mechanisms in semiconductors: (V) vacancy and (I) self-interstitial atoms. For the interstitialcy mechanism, it is assumed that the impurity-self-interstitial pair adopts a split interstitial configuration. The diffusive jump involves the correlated motion and rotation of the self-interstitial-impurity complex.

Impurity Diffusion:
Diffusion Coefficient

Note several Equation Errors in the online notes! All n_1's should be n_i's

Consider "simple" vacancy diffusion:

The diffusivity can be considered a superposition of all the diffusivity of all individual vacancy species (different charges):

$$D = D_{io} + \left[\frac{n}{n_i}\right]D^{1-} + \left[\frac{n}{n_1}\right]^2 D^{2-} + \left\{\left[\frac{n}{n_i}\right]^3 D^{3-} + \left[\frac{n}{n_i}\right]^4 D^{4-}\right\} + \left[\frac{p}{n_1}\right]D^{1+} + \left\{\left[\frac{p}{n_i}\right]^2 D^{2+} + \left[\frac{p}{n_i}\right]^3 D^{3+} + \left[\frac{p}{n_i}\right]^4 D^{4+}\right\}$$

Rarely are third and forth order terms important.

Each D value in the chart has the form:

$$D = D_o e^{\frac{-E_a}{kt}}$$

Table 3.2 Diffusion coefficients of common impurities in silicon and gallium arsenide

		Donors						Acceptors	
		$D_o^=$	$E_a^=$	D_o^-	E_a^-	D_{io}	E_{ia}	D_o^+	E_a^+
As in Si	D			12.0	4.05	0.066	3.44		
P in Si	D	44.0	4.37	4.4	4.0	3.9	3.66		
Sb in Si	D			15.0	4.08	0.21	3.65		
B in Si	A					0.037	3.46	0.41	3.46
Al in Si	A					1.39	3.41	2480	4.2
Ga in Si	A					0.37	3.39	28.5	3.92
S in GaAs	D					0.019	2.6		
Se in GaAs	D					3000	4.16		
Be in GaAs	A					7e − 6	1.2		
Ga in GaAs	I					0.1	3.2		
As in GaAs	I					0.7	5.6		

From Runyan and Bean [2] and references quoted therein. Donors are labeled with a "D", acceptors with an "A", and self-interstitials with an "I". All pre-exponentials are in cm²/sec and the activation energies are in electron volts.

Impurity Diffusion:
Diffusion Coefficient

Consider As vs B diffusion in Si:

Arsenic in Si is an important case where multiple diffusivity terms must be considered. At high concentrations of As, $n \gg n_i$. Thus, the first 2 terms must be used. The doping has enhanced the diffusion. At lower concentrations, $n < n_i$, only the intrinsic diffusivity term needs to be considered. *See example 3.1 in Campbell*. This concentration dependent diffusivity leads to a steep drop in the concentration when the concentration becomes lower than n_i. (Traffic jam analogy).
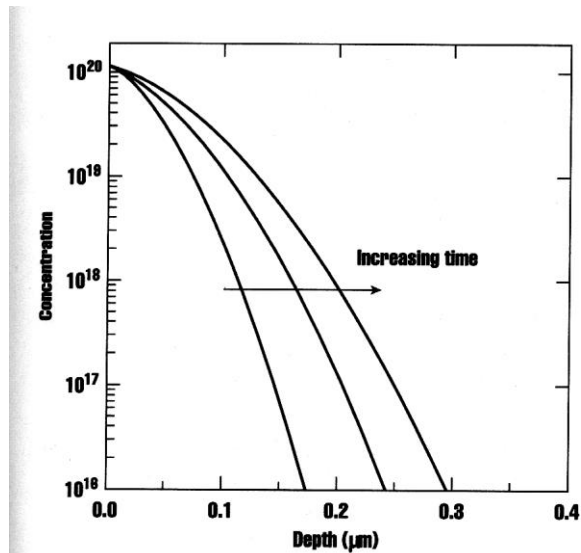
Figure 3-8 Typical profile for a high concentration boron diffusion.
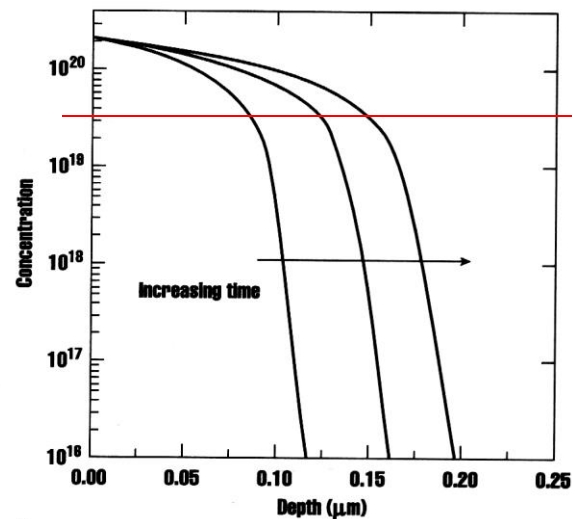
Figure 3-9 Typical profile for a high concentration arsenic diffusion.

n_i at elevated temperature: Diffusivity is higher for concentrations higher than n_i and lower for concentrations below n_i. This results in a more abrupt profile (preferred).

Impurity Diffusion:
Phosphorous Diffusion Coefficient

In reality, many diffusions are dominated by more than just vacancy reactions. Other defect complexes form. Consider P in Si.

At high concentrations, doubly charged vacancies, V^{2-}, combine with ionized phosphorous, P^+ to form a complex, $(PV)^-$

These dominate over singly charged vacancies. Thus,

$$D = D_i + D^{2-}\left[\frac{n}{n_i}\right]^2$$

At P-levels resulting in a fermi energy less than Ec-0.11 eV, the $(PV)^-$ pair disassociates according to,

$$(PV)^- = (PV)^0(unstable) + e^- \Leftrightarrow P^+ + V^-$$

This results in an excess of V^- resulting in a "kink region". This excess vacancy concentration leads to an enhanced diffusivity in the tail region.

Impurity Diffusion: Phosphorous Diffusion profile

Expected diffusion profile IF phosphorous was governed by simple intrinsic diffusion process.
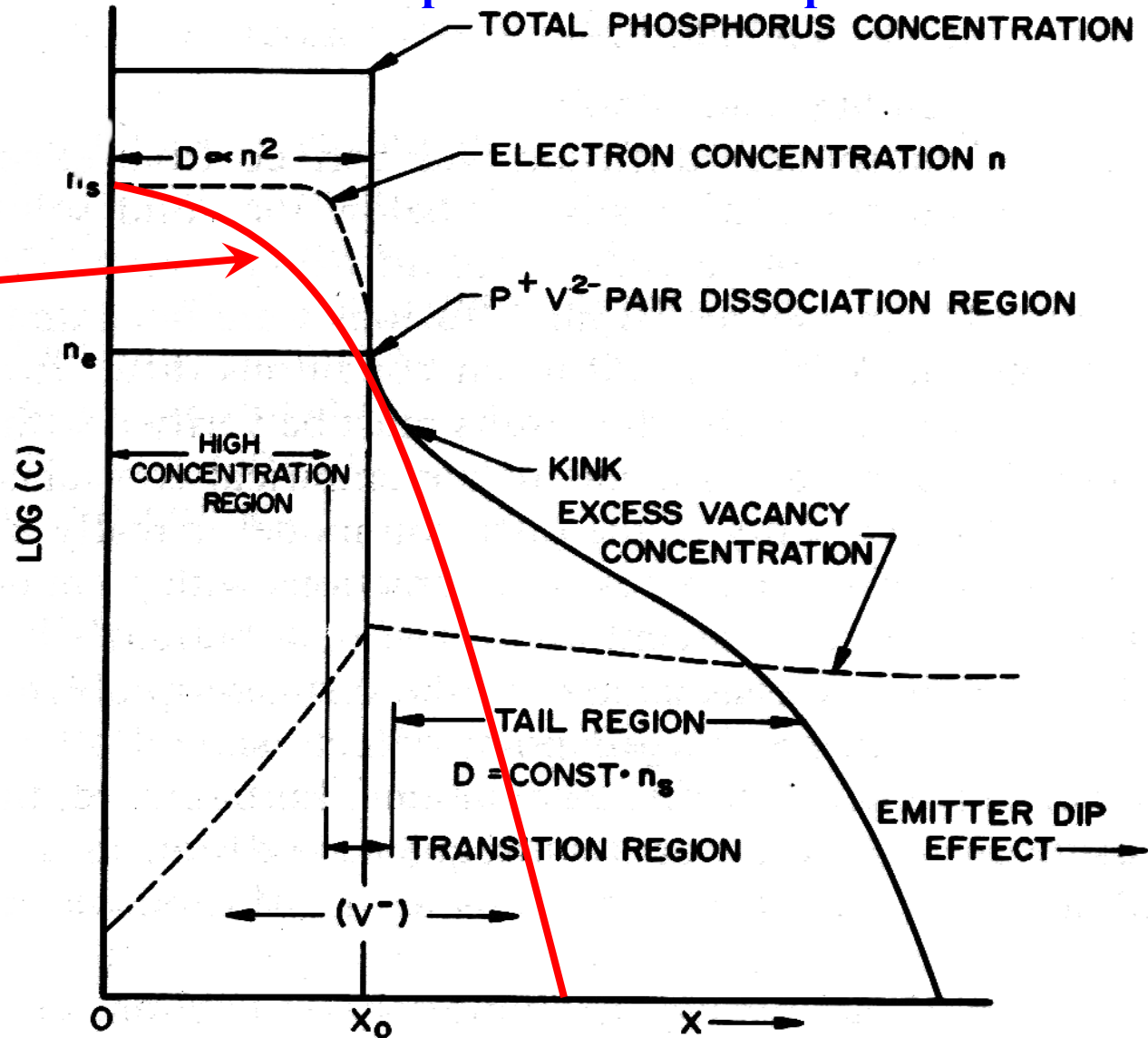
FIGURE 7
A model for phosphorus diffusion in silicon. (*After Fair, Ref. 17.*)

Solutions of the Basic Diffusion Equation: $\dfrac{\partial C(x,t)}{\partial t} = D\dfrac{\partial^2 C(x,t)}{\partial x^2}$

Many useful solutions exist in "The mathematics of Diffusion", 2nd Ed., John C. Frank (1975).

Three important cases exist:

1.) Infinite Source (non-depleting) Assumption (often termed "Predeposition")

Boundary conditions for equation 4 are C(z=0,t=0)=0, C(z=0,t>0)=C_S, and C(infinity, t)=0

Solution is,

$$C(z,t) = C_S\, erfc\left(\frac{z}{2\sqrt{Dt}}\right) \qquad , t > 0$$

where $\sqrt{Dt}$ is known as the characteristic diffusion length, C_S is the fixed surface concentration (most often set by the impurity solubility(and erfc is known as the complimentary error function.

The dose, Q(t), with units=[cm^{-2}] is defined as,

$$Q_T(t) = \int_0^\infty C(z,t)dz = \frac{2}{\sqrt{\pi}}C(0,t)\sqrt{Dt}$$

and the junction depth for a constant bulk concentration, C_B, is,

$$\mathrm{erf}(x) = \frac{2}{\sqrt{\pi}}\int_0^x e^{-t^2}\,\mathrm{dt}.$$

$$erfc(x) = 1 - erf(x)$$

Note: Often the erf is tabulated but not erfc

$$x_j = 2\sqrt{Dt}\, erfc^{-1}\left|\frac{C_B}{C_s}\right|$$

C

time

C_B

x_j

X
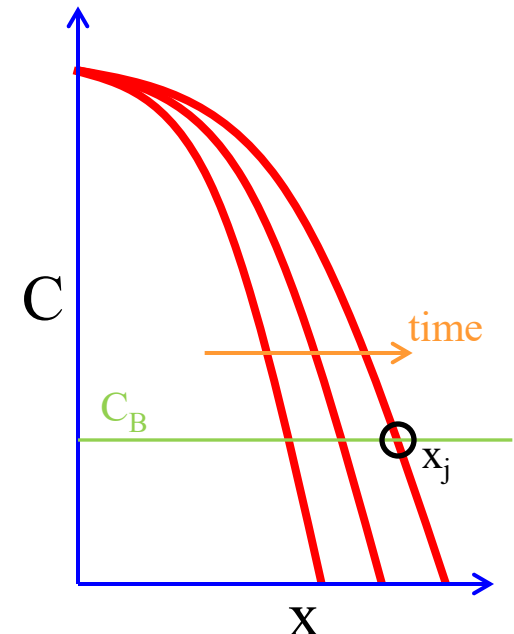
Solutions of the Basic Diffusion Equation: $\dfrac{\partial C(x,t)}{\partial t} = D\dfrac{\partial^2 C(x,t)}{\partial x^2}$

2.) Finite Source (depleting) Assumption (often termed "Drive in")

Boundary conditions for equation 4 are $C(z,0)=0$ for $z>0$, $dC(z=0,t)/dz=0$, and $C(z=\infty,t)=0$ and dose (area under the curves to the lower right), Q_T = constant.

Solution is a <u>Gaussian</u>,

$$C(z,t) = \frac{Q_T}{\sqrt{\pi Dt}}\, e^{\left(\frac{-z^2}{4Dt}\right)}$$

The surface concentration depletes as,

$$C_s = C(0,t) = \frac{Q_T}{\sqrt{\pi\, Dt}}$$

and the junction depth is,

$$x_j = \sqrt{4Dt\,\ln\!\left(\frac{Q_T}{C_B\sqrt{\pi\, Dt}}\right)}$$
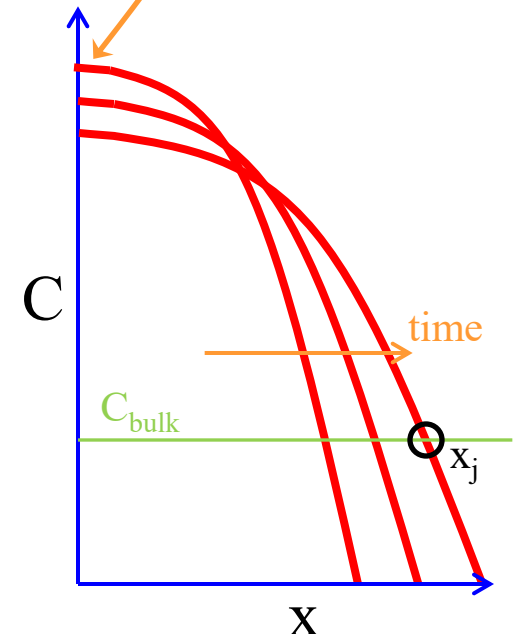
Solutions of the Basic Diffusion Equation:

Comparison of Infinite Source and Finite Source Diffusion

Infinite Source: Constant surface concentration @ solubility limit

Finite Source: Constant surface concentration slope but time varying concentration
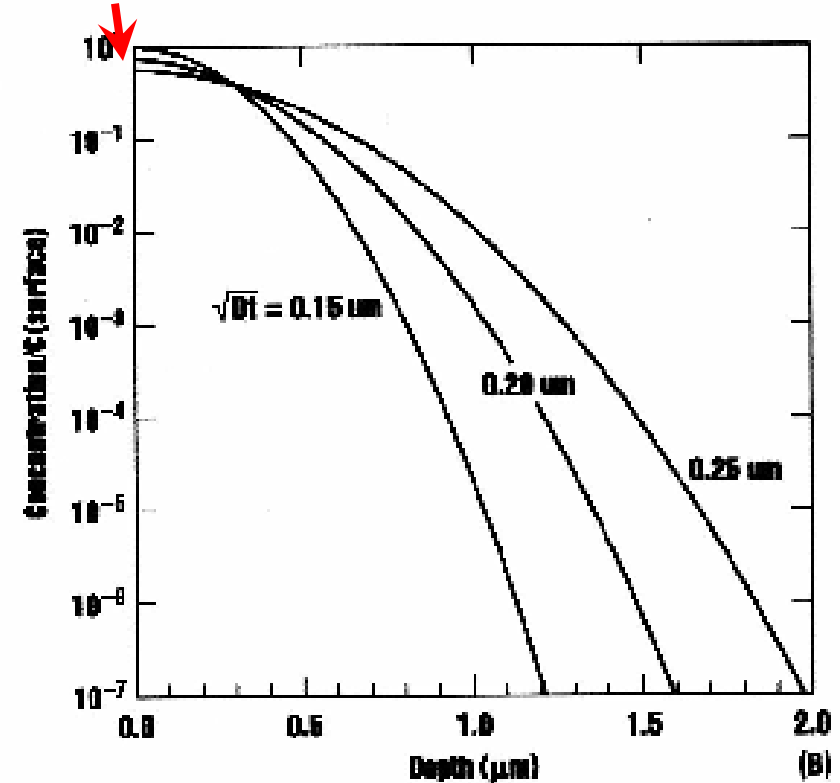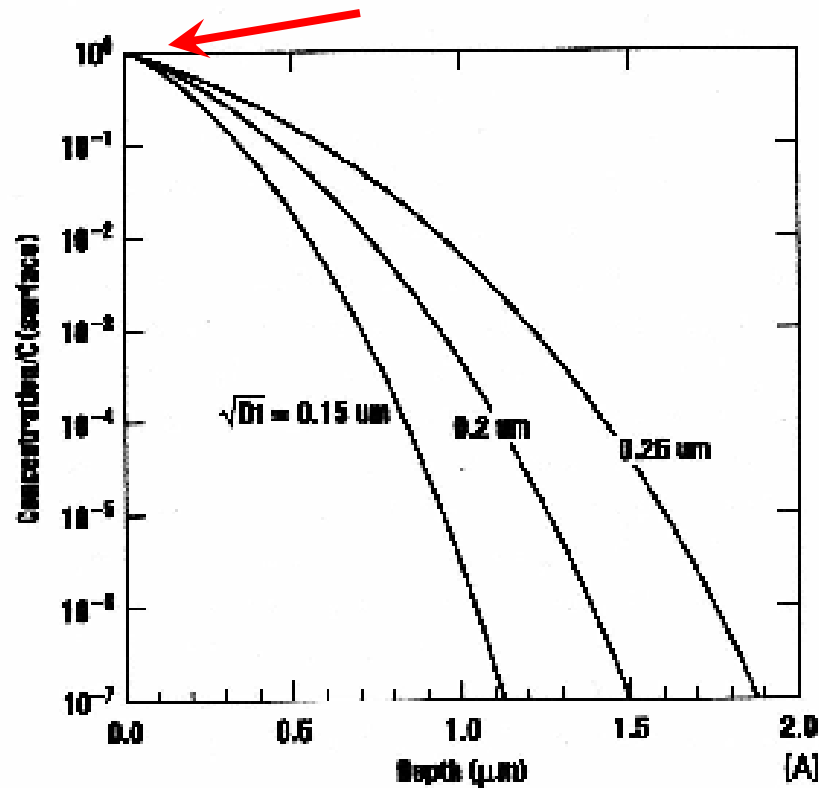
Figure 3-7 Concentration as a function of depth for (a) predeposition and (b) drive in diffusions for several values of the characteristic diffusion length.

Solutions of the Basic Diffusion Equation:

3.) Two step diffusion

1.) Predeposition with small $D_1(T)$ and t_1

2.) Turn off Impurity Source

3.) Oxidize the wafer

4.) Turn up the temperature (drive in) with large $D_2(T)$ and t_2

If $(D_1t_1)^{0.5} << (D_2t_2)^{0.5}$ ===> gaussian

If $(D_1t_1)^{0.5} >> (D_2t_2)^{0.5}$ ===> erfc

Fig. 4.20 Profiles for the two-step diffusion process.

Thus,

$$C(z, t_{1,} t_2) = \frac{2C(0, t_1)}{\pi} \int_0^U \frac{e^{-\beta(1+U^2)}}{1+U^2} dU \qquad U = \sqrt{\frac{D_1 t_t}{D_2 t_2}} \qquad \beta = \left[\frac{x}{2\sqrt{D_1 t_1 + D_2 t_2}} \right]^2$$

where the integral is known as the smith integral

Corrections to Diffusion Theory

Electric Field Enhancement:

The electric field created by the ionized impurities causes enhanced diffusion due to drift.

$$D \rightarrow D(1+\eta), where \, 0 < \eta < 1$$

Nitridization Enhancement/Retardation:

Exposure of the Si surface to NH_3 injects excess vacancies => enhancing vacancy mechanism diffusion (As), decreasing interstitialcy mechanism diffusion (P and B slow, less Si Interstitials due to trapping by vacancies)

Oxidation Enhancement/Retardation:

Exposure of the Si surface to an oxidizing process injects excess Si-Interstitials => enhancing interstitialcy mechanism diffusion (P and B), decreasing vacancy mechanism (As) diffusion

Since the oxidation rate is time dependent, the diffusivity becomes time dependent

$$D \rightarrow D + \alpha \left[\frac{dx_{oxide}}{dt} \right]^n$$

Where the second term is the oxidation induced diffusion coefficient change, x_{ox} is the thickness of the oxide, t is time, n=~0.3-0.6 for Si and α is a proportionality constant

Corrections to Diffusion Theory

Diffusion into other Materials:

Diffusion is enhanced in polycrystalline materials due to diffusion "down" grain boundaries.

Diffusion is slower in SiO_2. Thus, SiO_2 is an excellent high temperature diffusion mask.

Diffusion Characterization

Often times, the diffusion is characterized by the sheet resistance

$$R_s = \frac{1}{q \int\limits_0^\infty \mu(C)C(z)dz}$$

where μ is the concentration dependent mobility, and C is the "active" concentration (the concentration of dopants that have become ionized, often limited by degeneracy)

Supporting Information

TABLE 5
The diffusivity, solubility, and distribution coefficient at melting temperature of the fast diffusants in silicon

Element	Ref.	Diffusivity D_o (cm^2/s)	E (eV)	Solubility (cm^{-3})	Distribution coefficient
Li (25–1350°C)	41	2.3×10^{-3} to 9.4×10^{-4}	0.63– 0.78	Max. 7×10^{19} (1200°C)	10^{-2}
Na (800–1100°C)	41	1.6×10^{-3}	0.76	$(1-9) \times 10^{18}$ (600–1200°C)	
K (800–1100°C)	41	1.1×10^{-3}	0.76	$9 \times 10^{17} - 7 \times 10^{18}$ (600–1200°C)	
Cu (800–1100°C)	41	4.0×10^{-2}	1.0	$5 \times 10^{15} - 3 \times 10^{18}$ (600–1300°C)	4×10^{-4}
$(Cu)_i$ (300–700°C)	41	4.7×10^{-3}	0.43		
Ag (1100–1350°C)	41	2×10^{-3}	1.6	$6.5 \times 10^{15} - 2 \times 10^{17}$ (1200–1350°C)	1.1×10^{-4}
Au (800–1200°C) $(Au)_i$ $(Au)_s$ (700–1300°C)	41	1.1×10^{-3} 2.4×10^{-4} 2.8×10^{-3}	1.12 0.39 2.04	$5 \times 10^{14} - 5 \times 10^{16}$ (900–1300°C)	2.5×10^{-5}
Pt (800–1000°C)	42	$1.5-$ 1.7×10^{2}	2.22– 2.15	$4 \times 10^{16} - 5 \times 10^{17}$ (800–1000°C)	
Fe (1100–1250°C)	41	6.2×10^{-3}	0.87	$10^{13} - 5 \times 10^{16}$ (900–1300°C)	8×10^{-6}
Ni (450–800°C)	41	0.1	1.9	6×10^{18} (1200–1300°C)	$\sim 10^{-4}$
Cr (1100–1250°C)	43	0.01	1.0	$2 \times 10^{13} - 2.5 \times 10^{15}$ (900–1280°C)	
Co (900–1200°C)	44	9.2×10^{4}	2.8	Max. 2.5×10^{16} (1300°C)	8×10^{-6}
O_2 (700–1240°C)	45	7×10^{-2}	2.44	$1.5 \times 10^{17} - 2 \times 10^{18}$ (1000–1400°C)	5×10^{-1}
O_i (330–1250°C)	45	0.17	2.54		
H_2	41	9.4×10^{-3}	0.48	$2.4 \times 10^{21} \exp \frac{-1.86}{kT}$ at 1 atm	

Note: $(Cu)_i$ = interstitial copper, $(Au)_i$ = interstitial gold, $(Au)_s$ = substitutional gold, $(O)_i$ = interstitial (or isolated) oxygen.

TABLE 7
Diffusivities in SiO_2

Element	Ref.	D_o (cm^2/s)	E (eV)	$D(900°C)$ (cm^2/s)	C_s (cm^{-3})	Source and ambient
Boron	54	7.23×10^{-6}	2.38	4.4×10^{-16}	$10^{19}-$ 2×10^{20}	B_2O_3 vapor, $O_2 + N_2$
	54	1.23×10^{-4}	3.39	3.4×10^{-19}	6×10^{18}	B_2O_3 vapor, Ar
	54	3.16×10^{-4}	3.53	2.2×10^{-19}	$<3 \times 10^{20}$	Borosilicate
Gallium	54	1.04×10^{5}	4.17	1.3×10^{-13}	$\cdots$	Ga_2O_3 vapor, $H_2 + N_2 + H_2O$
Phosphorus	54	5.73×10^{-5}	2.30	7.7×10^{-15}	$8 \times 10^{20}-$ 10^{21}	P_2O_5 vapor, N_2
	55	1.86×10^{-1}	4.03	9.3×10^{-19}	$8 \times 10^{17}-$ 8×10^{19}	Phosphosilicate, N_2
Arsenic	56	67.25	4.7	4.5×10^{-19}	$<5 \times 10^{20}$	Ion implant, N_2
	56	3.7×10^{2}	3.7	4.8×10^{-18}	$<5 \times 10^{20}$	Ion implant, O_2
Antimony	57	3.7×10^{-11}	1.32	7.9×10^{-19}		Ion implant, N_2 or O_2
		1.2×10^{-7}	2.25	2.6×10^{-17}		Ion implant, O_2/H_2O
Hydrogen (H_2)	4	5.65×10^{-4}	0.446	7×10^{-6}		
Helium	4	3×10^{-4}	0.24	2.8×10^{-5}		
Water	4	10^{-6}	0.79	4×10^{-10}		
Oxygen	4	2.7×10^{-4}	1.16	2.8×10^{-9}		
Gold	4	8.2×10^{-10}	0.8	3×10^{-13}		
	4	1.52×10^{-7}	2.14	10^{-16}		
Platinum	4	1.2×10^{-13}	0.75	7.2×10^{-17}		
Sodium	4	6.9	1.3	1.8×10^{-5}		

Note: C_s = Surface concentration on silicon after diffusion from the specified source and ambient in the absence of an oxide barrier.

TABLE 8
Diffusion enhancement/retardation[70]

Elements	Oxidation	Oxynitridation	Direct nitridation
	Treatments		
P,B			
intrinsic	enhanced	enhanced	retarded
extrinsic	enhanced	enhanced	retarded
As			
intrinsic	enhanced	enhanced	enhanced
extrinsic	retarded or no effect	enhanced	enhanced
Sb*			
intrinsic	enhancement precedes retardation	enhancement precedes retardation	enhanced
Stacking faults	grow	grow	shrink

*The solid solubility of Sb is below 5×10^{19} cm^{-3}; all diffusions were under intrinsic conditions.

TABLE 6
Examples of diffusivities in polysilicon films

Elements	D_o (cm^2/s)	E (eV)	D (cm^2/s)	T (°C)	Ref.
As	8.6×10^4	3.9	2.4×10^{-14}	800	50
B	$(1.5-6) \times 10^{-3}$	2.4–2.5	9×10^{-14}	800	52
			4×10^{-14}	925	49
P			$(6.9-63) \times 10^{-13}$	1000	46
			$(1-7) \times 10^{-11}$	1200	46
Sb*	$D_g = 13.6 \pm \frac{60}{11}$	3.9 ± 0.2			53
	$D_{gb} = 812 \pm \frac{4000}{670}$	2.9 ± 0.2			53

* For the Sb diffusion, the diffusivities were determined from an assumed model. The D_g inside the grain and the D_{gb} along the grain boundary are given for temperatures between 930 and 1150 °C for D_g, and between 1050 and 1150 °C for D_{gb}.[53]

Table 4.5 Values of the Smith Integral[a]

U \ β	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1.0	1.1	1.2
0.1	0.09015	0.08155	0.07376	0.06672	0.06035	0.05459	0.04938	0.04467	0.04040	0.03655	0.03306	0.02990
0.2	0.17838	0.16119	0.14566	0.13162	0.11894	0.10748	0.09713	0.08777	0.07931	0.07167	0.06477	0.05853
0.3	0.26295	0.23723	0.21403	0.19310	0.17422	0.15719	0.14182	0.12795	0.11545	0.10416	0.09398	0.08479
0.4	0.34254	0.30837	0.27761	0.24993	0.22501	0.20259	0.18240	0.16422	0.14786	0.13314	0.11988	0.10794
0.5	0.41626	0.37374	0.33557	0.30132	0.27058	0.24299	0.21822	0.19599	0.17603	0.15812	0.14203	0.12759
0.6	0.48366	0.43290	0.38751	0.34692	0.31062	0.27814	0.24908	0.22308	0.19982	0.17900	0.16036	0.14368
0.7	0.54464	0.48580	0.43340	0.38673	0.34515	0.30809	0.27505	0.24562	0.21937	0.19596	0.17508	0.15645
0.8	0.59940	0.53264	0.47347	0.42100	0.37447	0.33317	0.29652	0.26398	0.23508	0.20940	0.18657	0.16628
0.9	0.64829	0.57380	0.50812	0.45017	0.39903	0.35385	0.31393	0.27864	0.24742	0.21979	0.19532	0.17365
1.0	0.69176	0.60975	0.53784	0.47475	0.41935	0.37066	0.32783	0.29013	0.25693	0.22765	0.20183	0.17903
1.1	0.73033	0.64100	0.56318	0.49529	0.43600	0.38415	0.33877	0.29900	0.26411	0.23348	0.20655	0.18286
1.2	0.76448	0.66808	0.58465	0.51232	0.44950	0.39486	0.34726	0.30574	0.26946	0.23772	0.20991	0.18553
1.3	0.79470	0.69148	0.60276	0.52634	0.46035	0.40327	0.35377	0.31078	0.27336	0.24074	0.21225	0.18734
1.4	0.82144	0.71164	0.61797	0.53781	0.46901	0.40979	0.35870	0.31449	0.27616	0.24286	0.21385	0.18855
1.5	0.84509	0.72899	0.63069	0.54714	0.47586	0.41482	0.36238	0.31720	0.27815	0.24431	0.21492	0.18933
1.6	0.86601	0.74388	0.64130	0.55469	0.48123	0.41865	0.36511	0.31914	0.27953	0.24530	0.21562	0.18983
1.7	0.88454	0.75666	0.65010	0.56076	0.48542	0.42153	0.36710	0.32051	0.28048	0.24595	0.21607	0.19014
1.8	0.90095	0.76759	0.65739	0.56562	0.48865	0.42369	0.36854	0.32147	0.28112	0.24638	0.21636	0.19033
1.9	0.91549	0.77693	0.66340	0.56948	0.49114	0.42529	0.36956	0.32213	0.28154	0.24665	0.21653	0.19045
2.0	0.92838	0.78491	0.66833	0.57254	0.49303	0.42646	0.37029	0.32258	0.28182	0.24682	0.21664	0.19051
2.5	0.97404	0.81009	0.68228	0.58029	0.49735	0.42887	0.37165	0.32335	0.28225	0.24707	0.21678	0.19059
3.0	0.99920	0.82094	0.68698	0.58234	0.49825	0.42928	0.37183	0.32343	0.28229	0.24708	0.21679	0.19059
∞	1.02834	0.82795	0.68892	0.58291	0.49843	0.42933	0.37184	0.32343	0.28229	0.24709	0.21679	0.19059

U \ β	1.3	1.4	1.5	1.6	1.7	1.8	1.9	2.0	2.5	3.0	4.0	5.0
0.1	0.02705	0.02446	0.02213	0.02002	0.01811	0.01638	0.01481	0.01340	0.00811	0.00491	0.00180	0.00066
0.2	0.05289	0.04779	0.04319	0.03903	0.03527	0.03187	0.02880	0.02603	0.01568	0.00945	0.00343	0.00125
0.3	0.07651	0.06903	0.06228	0.05620	0.05071	0.04575	0.04128	0.03725	0.02228	0.01333	0.00477	0.00171
0.4	0.09720	0.08752	0.07881	0.07097	0.06391	0.05756	0.05183	0.04668	0.02766	0.01640	0.00577	0.00204
0.5	0.11462	0.10297	0.09251	0.08312	0.07468	0.06711	0.06030	0.05419	0.03178	0.01866	0.00645	0.00224
0.6	0.12875	0.11538	0.10340	0.09268	0.08308	0.07448	0.06678	0.05988	0.03475	0.02021	0.00688	0.00236
0.7	0.13982	0.12499	0.11174	0.09992	0.08936	0.07993	0.07150	0.06398	0.03677	0.02120	0.00712	0.00242
0.8	0.14824	0.13219	0.11790	0.10519	0.09387	0.08379	0.07481	0.06680	0.03806	0.02180	0.00724	0.00245
0.9	0.15444	0.13741	0.12230	0.10889	0.09699	0.08642	0.07702	0.06867	0.03885	0.02213	0.00730	0.00245
1.0	0.15889	0.14109	0.12535	0.11141	0.09907	0.08814	0.07844	0.06985	0.03931	0.02231	0.00733	0.00246
1.1	0.16200	0.14361	0.12739	0.11307	0.10041	0.08923	0.07933	0.07056	0.03956	0.02240	0.00734	0.00246
1.2	0.16411	0.14529	0.12872	0.11412	0.10125	0.08989	0.07985	0.07098	0.03969	0.02244	0.00735	0.00246
1.3	0.16552	0.14638	0.12956	0.11478	0.10176	0.09028	0.08016	0.07122	0.03976	0.02246	0.00735	0.00246
1.4	0.16643	0.14706	0.13008	0.11517	0.10205	0.09051	0.08033	0.07134	0.03979	0.02247	0.00735	0.00246
1.5	0.16700	0.14749	0.13039	0.11540	0.10222	0.09063	0.08042	0.07141	0.03980	0.02247	0.00735	0.00246
1.6	0.16736	0.14774	0.13057	0.11552	0.10231	0.09070	0.08046	0.07144	0.03981	0.02247	0.00735	0.00246
1.7	0.16757	0.14789	0.13067	0.11559	0.10236	0.09073	0.08048	0.07146	0.03981	0.02247	0.00735	0.00246
1.8	0.16770	0.14797	0.13073	0.11563	0.10239	0.09075	0.08050	0.07147	0.03982	0.02247	0.00735	0.00246
1.9	0.16777	0.14802	0.13076	0.11565	0.10240	0.09075	0.08050	0.07147	0.03982	0.02247	0.00735	0.00246
2.0	0.16781	0.14804	0.13078	0.11566	0.10240	0.09076	0.08051	0.07147	0.03982	0.02247	0.00735	0.00246
2.5	0.16786	0.14807	0.13079	0.11567	0.10241	0.09076	0.08051	0.07147	—	—	—	—
3.0	0.16786	0.14807	0.13079	0.11567	0.10241	0.09076	0.08051	0.07147	—	—	—	—
∞	0.16786	0.14807	0.13079	0.11567	0.10241	0.09076	0.08051	0.07147	0.03982	0.02247	0.00735	0.00246

• From reference 23.

Supporting Information

Table A.1 Error Function erf z[a]

z	erf(z)	z	erf(z)	z	erf(z)	z	erf(z)
0.00	0.000 000	0.50	0.520 500	1.00	0.842 701	1.50	0.966 105
0.01	0.011 283	0.51	0.529 244	1.01	0.846 810	1.51	0.967 277
0.02	0.022 565	0.52	0.537 899	1.02	0.850 838	1.52	0.968 413
0.03	0.033 841	0.53	0.546 464	1.03	0.854 784	1.53	0.969 516
0.04	0.045 111	0.54	0.554 939	1.04	0.858 650	1.54	0.970 586
0.05	0.056 372	0.55	0.563 323	1.05	0.862 436	1.55	0.971 623
0.06	0.067 622	0.56	0.571 616	1.06	0.866 144	1.56	0.972 628
0.07	0.078 858	0.57	0.579 816	1.07	0.869 773	1.57	0.973 603
0.08	0.090 078	0.58	0.587 923	1.08	0.873 326	1.58	0.974 547
0.09	0.101 281	0.59	0.595 936	1.09	0.876 803	1.59	0.975 462
0.10	0.112 463	0.60	0.603 856	1.10	0.880 205	1.60	0.976 348
0.11	0.123 623	0.61	0.611 681	1.11	0.883 533	1.61	0.977 207
0.12	0.134 758	0.62	0.619 411	1.12	0.886 788	1.62	0.978 038
0.13	0.145 867	0.63	0.627 046	1.13	0.889 971	1.63	0.978 843
0.14	0.156 947	0.64	0.634 586	1.14	0.893 082	1.64	0.979 622
0.15	0.167 996	0.65	0.642 029	1.15	0.896 124	1.65	0.980 376
0.16	0.179 012	0.66	0.649 377	1.16	0.899 096	1.66	0.981 105
0.17	0.189 992	0.67	0.656 628	1.17	0.902 000	1.67	0.981 810
0.18	0.200 936	0.68	0.663 782	1.18	0.904 837	1.68	0.982 493
0.19	0.211 840	0.69	0.670 840	1.19	0.907 608	1.69	0.983 153
0.20	0.222 703	0.70	0.677 801	1.20	0.910 314	1.70	0.983 790
0.21	0.233 522	0.71	0.684 666	1.21	0.912 956	1.71	0.984 407
0.22	0.244 296	0.72	0.691 433	1.22	0.915 534	1.72	0.985 003
0.23	0.255 023	0.73	0.698 104	1.23	0.918 050	1.73	0.985 578
0.24	0.265 700	0.74	0.704 678	1.24	0.920 505	1.74	0.986 135
0.25	0.276 326	0.75	0.711 156	1.25	0.922 900	1.75	0.986 672
0.26	0.286 900	0.76	0.717 537	1.26	0.925 236	1.76	0.987 190
0.27	0.297 418	0.77	0.723 822	1.27	0.927 514	1.77	0.987 691
0.28	0.307 880	0.78	0.730 010	1.28	0.929 734	1.78	0.988 174
0.29	0.318 283	0.79	0.736 103	1.29	0.931 899	1.79	0.988 641
0.30	0.328 627	0.80	0.742 101	1.30	0.934 008	1.80	0.989 091
0.31	0.338 908	0.81	0.748 003	1.31	0.936 063	1.81	0.989 525
0.32	0.349 126	0.82	0.753 811	1.32	0.938 065	1.82	0.989 943
0.33	0.359 279	0.83	0.759 524	1.33	0.940 015	1.83	0.990 347
0.34	0.369 365	0.84	0.765 143	1.34	0.941 914	1.84	0.990 736
0.35	0.379 382	0.85	0.770 668	1.35	0.943 762	1.85	0.991 111
0.36	0.389 330	0.86	0.776 100	1.36	0.945 561	1.86	0.991 472
0.37	0.399 206	0.87	0.781 440	1.37	0.947 312	1.87	0.991 821
0.38	0.409 009	0.88	0.786 687	1.38	0.949 016	1.88	0.992 156
0.39	0.418 739	0.89	0.791 843	1.39	0.950 673	1.89	0.992 479
0.40	0.428 392	0.90	0.796 908	1.40	0.952 285	1.90	0.992 790
0.41	0.437 969	0.91	0.801 883	1.41	0.953 852	1.91	0.993 090
0.42	0.447 468	0.92	0.806 768	1.42	0.955 376	1.92	0.993 378
0.43	0.456 887	0.93	0.811 564	1.43	0.956 857	1.93	0.993 656
0.44	0.466 225	0.94	0.816 271	1.44	0.958 297	1.94	0.993 923
0.45	0.475 482	0.95	0.820 891	1.45	0.959 695	1.95	0.994 179
0.46	0.484 655	0.96	0.825 424	1.46	0.961 054	1.96	0.994 426
0.47	0.493 745	0.97	0.829 870	1.47	0.962 373	1.97	0.994 664
0.48	0.502 750	0.98	0.834 232	1.48	0.963 654	1.98	0.994 892
0.49	0.511 668	0.99	0.838 508	1.49	0.964 898	1.99	0.995 111

z	erf(z)	z	erf(z)	z	erf(z)	z	erf(z)
2.00	0.995 322	2.50	0.999 593	3.00	0.999 977 91	3.50	0.999 999 257
2.01	0.995 525	2.51	0.999 614	3.01	0.999 979 26	3.51	0.999 999 309
2.02	0.995 719	2.52	9.999 634	3.02	0.999 980 53	3.52	0.999 999 358
2.03	0.995 906	2.53	0.999 654	3.03	0.999 981 73	3.53	0.999 999 403
2.04	0.996 086	2.54	0.999 672	3.04	0.999 982 86	3.54	0.999 999 445
2.05	0.996 258	2.55	0.999 689	3.05	0.999 983 92	3.55	0.999 999 485
2.06	0.996 423	2.56	0.999 706	3.06	0.999 984 92	3.56	0.999 999 521
2.07	0.996 582	2.57	0.999 722	3.07	0.999 985 86	3.57	0.999 999 555
2.08	0.996 734	2.58	0.999 736	3.08	0.999 986 74	3.58	0.999 999 587
2.09	0.996 880	2.59	0.999 751	3.09	0.999 987 57	3.59	0.999 999 617
2.10	0.997 021	2.60	0.999 764	3.10	0.999 988 35	3.60	0.999 999 644
2.11	0.997 155	2.61	0.999 777	3.11	0.999 989 08	3.61	0.999 999 670
2.12	0.997 284	2.62	0.999 789	3.12	0.999 989 77	3.62	0.999 999 694
2.13	0.997 407	2.63	0.999 800	3.13	0.999 990 42	3.63	0.999 999 716
2.14	0.997 525	2.64	0.999 811	3.14	0.999 991 03	3.64	0.999 999 736
2.15	0.997 639	2.65	0.999 822	3.15	0.999 991 60	3.65	0.999 999 756
2.16	0.997 747	2.66	0.999 831	3.16	0.999 992 14	3.66	0.999 999 773
2.17	0.997 851	2.67	0.999 841	3.17	0.999 992 64	3.67	0.999 999 790
2.18	0.997 951	2.68	0.999 849	3.18	0.999 993 11	3.68	0.999 999 805
2.19	0.998 046	2.69	0.999 858	3.19	0.999 993 56	3.69	0.999 999 820
2.20	0.998 137	2.70	0.999 866	3.20	0.999 993 97	3.70	0.999 999 833
2.21	0.998 224	2.71	0.999 873	3.21	0.999 994 36	3.71	0.999 999 845
2.22	0.998 308	2.72	0.999 880	3.22	0.999 994 73	3.72	0.999 999 857
2.23	0.998 388	2.73	0.999 887	3.23	0.999 995 07	3.73	0.999 999 867
2.24	0.998 464	2.74	0.999 893	3.24	0.999 995 40	3.74	0.999 999 877
2.25	0.998 537	2.75	0.999 899	3.25	0.999 995 70	3.75	0.999 999 886
2.26	0.998 607	2.76	0.999 905	3.26	0.999 995 98	3.76	0.999 999 895
2.27	0.998 674	2.77	0.999 910	3.27	0.999 996 24	3.77	0.999 999 903
2.28	0.998 738	2.78	0.999 916	3.28	0.999 996 49	3.78	0.999 999 910
2.29	0.998 799	2.79	0.999 920	3.29	0.999 996 72	3.79	0.999 999 917
2.30	0.998 857	2.80	0.999 925	3.30	0.999 996 94	3.80	0.999 999 923
2.31	0.998 912	2.81	0.999 929	3.31	0.999 997 15	3.81	0.999 999 929
2.32	0.998 966	2.82	0.999 933	3.32	0.999 997 34	3.82	0.999 999 934
2.33	0.999 016	2.83	0.999 937	3.33	0.999 997 51	3.83	0.999 999 939
2.34	0.999 065	2.84	0.999 941	3.34	0.999 997 68	3.84	0.999 999 944
2.35	0.999 111	2.85	0.999 944	3.35	0.999 997 838	3.85	0.999 999 948
2.36	0.999 155	2.86	0.999 948	3.36	0.999 997 983	3.86	0.999 999 952
2.37	0.999 197	2.87	0.999 951	3.37	0.999 998 120	3.87	0.999 999 956
2.38	0.999 237	2.88	0.999 954	3.38	0.999 998 247	3.88	0.999 999 959
2.39	0.999 275	2.89	0.999 956	3.39	0.999 998 367	3.89	0.999 999 962
2.40	0.999 311	2.90	0.999 959	3.40	0.999 998 478	3.90	0.999 999 965
2.41	0.999 346	2.91	0.999 961	3.41	0.999 998 582	3.91	0.999 999 968
2.42	0.999 379	2.92	0.999 964	3.42	0.999 998 679	3.92	0.999 999 970
2.43	0.999 411	2.93	0.999 966	3.43	0.999 998 770	3.93	0.999 999 973
2.44	0.999 441	2.94	0.999 968	3.44	0.999 998 855	3.94	0.999 999 975
2.45	0.999 469	2.95	0.999 970	3.45	0.999 998 934	3.95	0.999 999 977
2.46	0.999 497	2.96	0.999 972	3.46	0.999 999 008	3.96	0.999 999 979
2.47	0.999 523	2.97	0.999 973	3.47	0.999 999 077	3.97	0.999 999 980
2.48	0.999 547	2.98	0.999 975	3.48	0.999 999 141	3.98	0.999 999 982
2.49	0.999 571	2.99	0.999 976	3.49	0.999 999 201	3.99	0.999 999 983

[a] For a more complete table, see L. J. Comrie, *Chambers Six Figure Mathematical Tables*, Vol. 2, W. & R. Chambers, Edinburgh, 1949.