

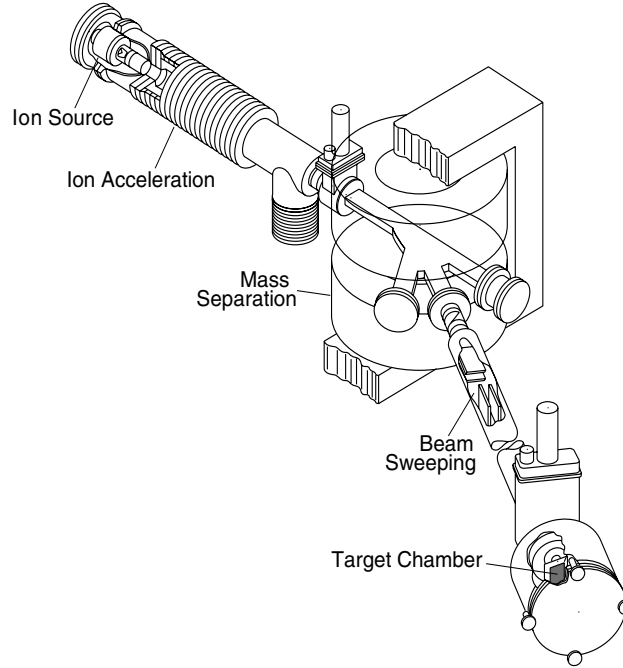
# 1 General Features and Fundamental Concepts

## 1.1 Introduction

Ion beam processing of materials results from the introduction of atoms into the surface layer of a solid substrate by bombardment of the solid with ions in the electron-volt to mega-electron-volt energy range. The solid-state aspects are particularly broad because of the range of physical properties that are sensitive to the presence of a trace amount of foreign atoms. Mechanical, electrical, optical, magnetic, and superconducting properties all are affected by, and indeed may even be dominated by, the presence of such foreign atoms. The use of energetic ions affords the possibility of introducing a wide range of atomic species, independent of thermodynamic factors, thus making it possible to obtain impurity concentrations and distributions of particular interest; in many cases, these distributions would not otherwise be attainable.

Recent interest in ion beam processing has focused on studies of ion implantation, ion beam mixing, ion-induced phase transformations, and ion beam deposition. These interests have been stimulated by the possibilities of synthesizing novel materials with potential applications in the semiconductor, tribological, corrosion, and optical fields.

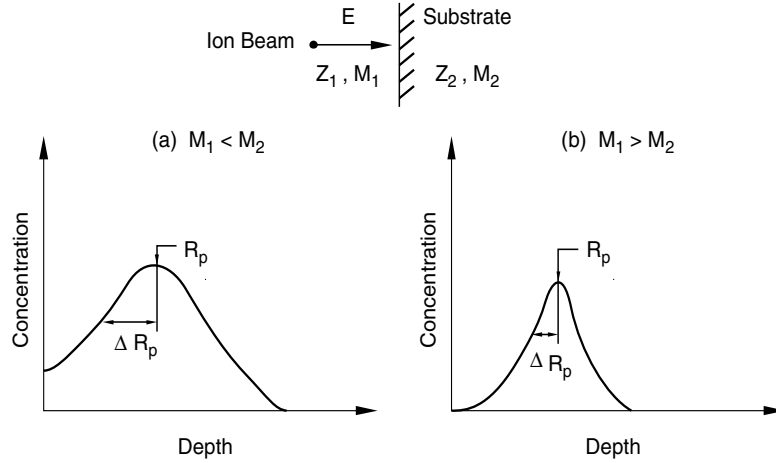
Ion beam processing provides an alternative and non-equilibrium method of introducing dopant atoms into the lattice. In typical applications, a beam of dopant ions is accelerated through a potential of 10–100 kV. The implantation system shown in Fig. 1.1 illustrates the basic elements required in this technique: ion source, acceleration column, mass-separator, and target chamber. With different types of ion sources available, a wide variety of beams may be produced with sufficient intensity for implantation purposes for integrated circuit technology;  $10^{14}$ – $10^{15}$  ions  $\text{cm}^{-2}$  (less than a ‘monolayer’; see Sect. 1.4) is a representative ion dose. *Ion dose* is defined as the number of ions  $\text{cm}^{-2}$  implanted into the sample. Alternatively, the term *fluence* is used instead of dose. The ion beam current density is expressed in units of  $\text{A cm}^{-2}$ . The dose rate or flux is given in units of ions  $\text{s}^{-1} \text{cm}^{-2}$ .



**Fig. 1.1.** Schematic drawing of an ion implantation system. A mass-separating magnet is used to select the ion species (elements and isotopes) of interest. Beam-sweeping facilities are required for large-area uniform implantations

## 1.2 Range Distributions

One of the most important considerations in any description of ion–solid interactions is the depth (range) distribution of the implanted ions. A large amount of experimental and theoretical work has been devoted to the task of understanding the energy-loss processes that govern the range distribution, and it is now possible to predict fairly accurately most of the factors involved. For example, a typical range distribution in an amorphous substrate from monoenergetic ions at moderate ion doses is approximately Gaussian in shape and may therefore be characterized by a projected range,  $R_p$ , and a straggling,  $\Delta R_p$ , about this mean value, as depicted in Fig. 1.2. The notation uses  $Z$  and  $M$  for atomic number and atomic mass, respectively, with subscript 1 denoting the incident ions ( $Z_1, M_1$ ) and subscript 2 denoting the ion-bombarded sample (or target). By convention, the energy of the incident ion is denoted by  $E_0$  or by  $E$  without a subscript.

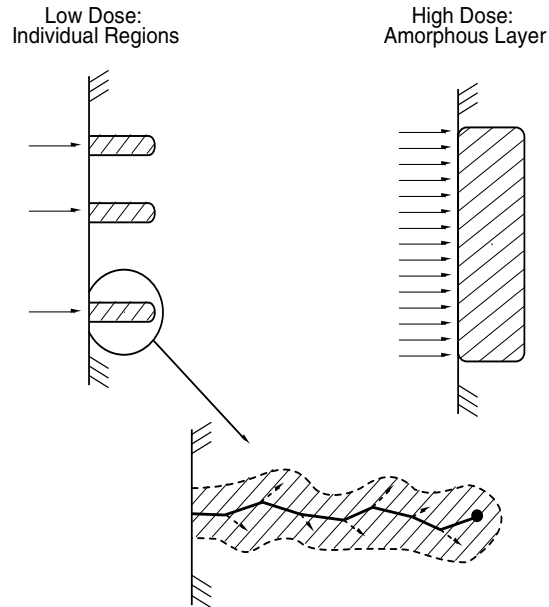


**Fig. 1.2.** The depth distribution of implanted atoms in an amorphous target for the cases in which the ion mass is (a) less than the mass of the substrate atoms or (b) greater than the mass of the substrate atoms. To a first approximation, the mean depth,  $R_p$ , depends on ion mass,  $M_1$ , and incident energy,  $E$ , whereas the relative width,  $\Delta R_p/R_p$ , of the distribution depends primarily on the ratio between ion mass and the mass of the substrate ion,  $M_2$

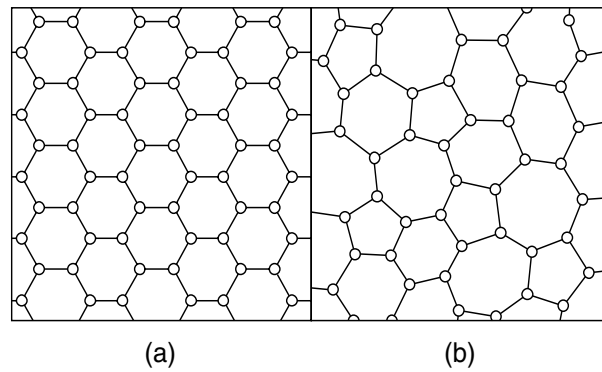
## 1.3 Lattice Disorder

Lattice disorder and radiation-damage effects are produced in the substrate by the incident ion. As an implanted ion slows down and comes to rest, it has many violent collisions with lattice atoms, displacing them from their lattice sites. These displaced atoms can in turn displace others, and the net result is the production of a highly disordered region around the path of the ion, as shown schematically in Fig. 1.3 for the case of a heavy implanted atom at typically 10–100 keV. At sufficiently high doses, these individual disordered regions may overlap, and an amorphous or metastable crystalline layer may form.

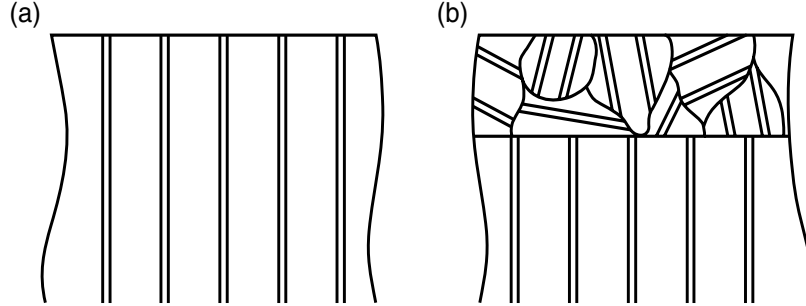
Figure 1.4 shows the schematic atomic arrangement for a crystalline solid (a) and an amorphous solid (b). A crystalline solid has long-range atomic order; an amorphous solid has short-range order (the order among the nearest neighbors) but no long-range order. In a single-crystal, the entire sample is composed of atoms placed on well-defined planes and rows. Figure 1.5a shows a side view of a single-crystal, in which the planes of atoms are depicted by parallel pairs of lines. A polycrystalline sample is made of small single-crystal regions called crystallites, the planes and atomic rows of which are misaligned with respect to those in neighboring crystallites. A polycrystalline layer on a single-crystal substrate is shown in Fig. 1.5b.



**Fig. 1.3.** A schematic representation of the disorder produced in room-temperature implantations of heavy ions at energies of 10–100 keV. At low doses, the highly disordered regions around the tracks of the ions are spatially separated from each other. The volume of the disordered region is determined primarily by the stopping point of the ion and the range of the displaced lattice atoms (*dashed arrows*). At high doses, the disordered regions can overlap to form an amorphous layer



**Fig. 1.4.** Schematic atomic arrangement of (a) a crystalline solid and (b) an amorphous solid



**Fig. 1.5.** Schematic representation for (a) a single-crystal with crystallographic planes perpendicular to the surface and (b) a polycrystalline layer on a single-crystal

## 1.4 Atomic and Planar Densities

To understand the description of ion implantation and ion doses, one must know the atomic density interplanar distance between planes and the number of atoms  $\text{cm}^{-2}$  on a given plane. In cubic systems with an atomic density of  $N$  atoms  $\text{cm}^{-3}$ , the crystal lattice parameter,  $a_c$ , is given by

$$a_c = \left( \frac{\text{atoms/unit cell}}{N} \right)^{1/3}, \quad (1.1)$$

where, for systems with one atom per lattice point, there are four atoms per unit cell for a face-centered-cubic lattice (Al, Ag, Au, Pd, Pt) and there are eight for the common semiconductors germanium (Ge) and silicon (Si), which have the diamond cubic structure. Aluminum has an atomic density of  $6.02 \times 10^{22}$  atoms  $\text{cm}^{-3}$ , so that the lattice parameter is

$$a_c = \left( \frac{4}{6.02 \times 10^{22}} \right)^{1/3} = 4.05 \times 10^{-8} \text{ cm}. \quad (1.2)$$

The atomic volume can be calculated without the use of crystallography. The atomic density  $N$  of atoms  $\text{cm}^{-3}$  is given by

$$N = \frac{N_A}{A} \rho, \quad (1.3)$$

where  $N_A$  is Avogadro's number,  $\rho$  is the mass density in  $\text{g cm}^{-3}$ , and  $A$  is the atomic mass number. Taking Al as an example, where  $\rho$  is  $2.7 \text{ g cm}^{-3}$  and  $A$  is 27, the atomic density is  $N = (6.02 \times 10^{23} \times 2.70)/27 = 6.02 \times 10^{22} \text{ atoms cm}^{-3}$ . The semiconductors Ge and Si have atomic densities of about  $4.4 \times 10^{22}$  and  $5.0 \times 10^{22} \text{ atoms cm}^{-3}$ , respectively. Metals such as Co, Ni, and Cu have densities of about  $9 \times 10^{22} \text{ atoms cm}^{-3}$ . The volume  $\Omega_V$  occupied by an atom is given by

$$\Omega_V = \frac{1}{N} \quad (1.4)$$

with a typical value of  $20 \times 10^{-24} \text{ cm}^3$ .

The average areal density of a monolayer,  $N_s \text{ atoms cm}^{-2}$ , also can be estimated without the use of crystallography by taking the atomic density  $N$  to the  $2/3$  power.

$$N_s \cong N^{2/3}. \quad (1.5)$$

Equation (1.5) gives the average areal density of one monolayer for a material with an atomic density  $N$ .

## 1.5 Energy and Particles

In the SI (or MKS) system of units, the joule (J) is a unit of energy, but the electron-volt (eV) is the traditional unit used in ion–solid interactions: we can define 1 eV as the kinetic energy gained by an electron accelerated through a potential difference of 1 V. The charge on the electron is  $1.602 \times 10^{-19} \text{ C}$ , and a joule is a Coulomb-volt, so that the relationship between these units is given by

$$1 \text{ eV} = 1.602 \times 10^{-19} \text{ J}. \quad (1.6)$$

Commonly used multiples of the electron-volt are the kilo-electron-volt ( $10^3 \text{ eV}$ ) and mega-electron-volt ( $10^6 \text{ eV}$ ).

In ion–solid interactions it is convenient to use cgs units rather than SI units in relations involving the charge on the electron. The usefulness of cgs units is clear when considering the Coulomb force between two charged particles with  $Z_1$  and  $Z_2$  units of electronic charge separated by a distance  $r$

$$F = \frac{Z_1 Z_2 e^2 k_c}{r^2}, \quad (1.7)$$

where the Coulomb law constant  $k_c = \frac{1}{4} \pi \epsilon_0 = 8.988 \times 10^9 \text{ m F}^{-1}$  in the SI system (where  $1 \text{ F} \equiv 1 \text{ A s V}^{-1}$ ) and is equal to unity in the cgs system.

The conversion factor follows from:

$$e^2 k_c = (1.6 \times 10^{-19} \text{ C})^2 \times 8.988 \times 10^9 \text{ m F}^{-1} = 2.3 \times 10^{-28} \text{ C}^2 \text{ m F}^{-1}.$$

The conversions  $1 \text{ C} \equiv 1 \text{ A s}$  and  $1 \text{ J} \equiv 1 \text{ C V}$  lead to the units of the farad:

$$1 \text{ F} \equiv 1 \text{ A s V}^{-1},$$

so that

$$1 \text{ C}^2 \text{ m F}^{-1} \equiv 1 \text{ C}^2 \text{ V m (A s)}^{-1} \equiv 1 \text{ J m} \equiv 10^9 \text{ J nm} \equiv \frac{10^9 \text{ J nm}}{(1.6 \times 10^{-19} \text{ J eV}^{-1})} = \frac{10^{28}}{1.6} \text{ eV nm}$$

and

$$e^2 k_c = 2.31 \times 10^{-28} \text{ C}^2 \text{ m F}^{-1} = \frac{2.31}{1.6} \text{ eV nm} = 1.44 \text{ eV nm}.$$

In this book we will follow the cgs units for  $e^2$  with  $k_c = 1$ , so that

$$e^2 = 1.44 \text{ eV nm}. \quad (1.8)$$

Each nucleus is characterized by a definite atomic number  $Z$  and mass number  $A$ ; for clarity, we use the symbol  $M$  to denote the atomic mass in kinematic equations. The atomic number  $Z$  is the number of protons, and hence the number of electrons, in the neutral atom; it reflects the atomic properties of the atom. The mass number gives the number of nucleons (protons and neutrons); isotopes are nuclei (often called nuclides) with the same  $Z$  and different  $A$ . The current practice is to represent each nucleus by the chemical name with the mass number as a superscript, e.g.,  $^{12}\text{C}$ . The chemical atomic weight (or atomic mass) of elements as listed in the periodic table gives the average mass, i.e., the average of the stable isotopes weighted by their abundance. Carbon, for example, has an atomic weight of 12.011, which reflects the 1.1% abundance of  $^{13}\text{C}$ .

The masses of particles may be expressed as given in Table 1.1 in terms of energy through the Einstein relation

$$E = Mc^2, \quad (1.9)$$

**Table 1.1.** Mass energies of particles and light nuclei

Particle	Symbol	Atomic mass (u)	Mass ( $10^{-27}$ kg)	Mass energy (MeV)
Electron	e or $e^-$	0.000549	$9.1095 \times 10^{-4}$	0.511
Proton	p or $^1\text{H}^+$	1.007276	1.6726	938.3
Atomic mass unit (amu)	u	1.00000	1.6606	931.7
Neutron	n	1.008665	1.6747	939.6
Deuteron	D or $^2\text{H}^+$	2.01410	3.3429	1875.6
Alpha	$\alpha$ or $^4\text{He}^{2+}$	4.00260	6.6435	3727.4

which associates 1 J of energy with  $1/c^2$  of mass, where  $c$  is the velocity of light,  $c = 2.998 \times 10^8 \text{ m s}^{-1}$ . The mass of an electron,  $m_e$ , is  $9.11 \times 10^{-31} \text{ kg}$ , which is equivalent to an energy

$$E = (9.11 \times 10^{-31} \text{ kg})(2.998 \times 10^8 \text{ m s}^{-1})^2 = 8.188 \times 10^{-14} \text{ J} = 0.511 \text{ MeV.} \quad (1.10)$$

The Einstein relation is also useful when calculating the velocity,  $v$ , of an ion of mass  $M$  and energy  $E$ ,

$$v = \left( \frac{2E}{M} \right)^{1/2} = c \left( \frac{2E}{Mc^2} \right)^{1/2}. \quad (1.11)$$

For example, the velocity of a 2 MeV  $^4\text{He}$  ion is

$$v = 3 \times 10^8 \text{ m s}^{-1} \left( \frac{2 \times 2 \times 10^6 (\text{eV})}{3,727 \times 10^6 (\text{eV})} \right)^{1/2} = 9.8 \times 10^6 \text{ m s}^{-1}.$$

## 1.6 The Bohr Velocity and Radius

The Bohr atom provides useful relations for simple estimates of atomic parameters. The Bohr radius is defined as the distance of the ground state electron from the nucleus in a hydrogen atom. The Bohr radius of the hydrogen atom is given by



$$a_0 = \frac{\hbar^2}{m_e e^2} = 0.5292 \times 10^{-8} \text{ cm} = 0.05292 \text{ nm} \quad (1.12)$$

and the Bohr velocity of the electron in this orbit is

$$v_0 = \frac{\hbar}{m_e a_0} = \frac{e^2}{\hbar} = 2.188 \times 10^8 \text{ cm s}^{-1}, \quad (1.13)$$

where  $\hbar = h / 2\pi$  with Planck's constant  $h = 4.136 \times 10^{-15} \text{ eV s}$ . For comparison with the Bohr radius, the radius of a nucleus is given by the empirical formula

$$R = R_0 A^{1/3}, \quad (1.14)$$

where  $A$  is the mass number and  $R_0$  is a constant equal to  $1.4 \times 10^{-13} \text{ cm}$ . The nuclear radius is about four orders of magnitude smaller than the Bohr radius.

## Suggested Reading

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## Problems

- 1.1 Aluminum is a face-centered-cubic with a mass density of  $2.70 \text{ g cm}^{-3}$   
 (a) Calculate the atomic density using (1.3)

- (b) Calculate the average areal density using (1.5)
- (c) What is the atomic volume?
- 1.2 For the canonical value of  $10^{15}$  atoms  $\text{cm}^{-2}$  in a monolayer on a cubic crystal, estimate
  - (a) The bulk density
  - (b) The volume  $\Omega_V$  occupied by an atom
- 1.3 Nickel is a face-centered-cubic metal with an atomic density of  $9.14 \times 10^{22}$  atoms  $\text{cm}^{-3}$ , an atomic weight of 8.7, and density of  $8.91 \text{ g cm}^{-3}$ 
  - (a) What is the lattice parameter,  $a_c$ , and the atomic volume,  $\Omega_V$ ?
- 1.4 Silicon has a diamond cubic lattice structure with an atomic density of  $5 \times 10^{22}$  atoms  $\text{cm}^{-3}$ , an atomic weight of 28.09 and a density of  $2.33 \text{ g cm}^{-3}$ 
  - (a) What are silicon's lattice parameter and atomic volume,  $\Omega_V$ ?
- 1.5 Calculate the energy in eV of a proton moving at the Bohr velocity. What is the velocity of a 35 keV A s ion?

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