

Introduction to Space Charge Effects in Semiconductors

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Space Charges in Insulators

Summary. The space charges in insulators directly determine the built-in field and electron energy distribution, as long as carrier transport can be neglected.

In this chapter we present a few arbitrarily introduced space-charge profiles and point out some of the basic resulting field and band edge distributions with consequences to device applications.

1.1 Basic Electrostatic Relations

The basic electrostatic relations connect charges, forces, fields and potential with each other under static (as opposed to dynamic) conditions.

We start from the *Coulomb relation* describing the force between two fixed point charges, e_1 and e_2 .

$$\mathcal{F} = c_u \frac{e_1 e_2}{r_0^2} \quad (1.1)$$

with r_0 as the distance between the two charges. The units-related constant c_u (*in vacuo*) is set, in the rational four-parameter system used in this book, to $c_u = 1/(4\pi\epsilon_0)$ with the vacuum permittivity $\epsilon_0 = 8.8543 \times 10^{-14}$ (AsV⁻¹cm⁻¹ = Farad cm⁻¹). For $e_1 = e_2 = e$ one obtains¹

$$\mathcal{F} = \frac{e^2}{4\pi\epsilon_0 r_0^2} = \begin{cases} 2.3 \times 10^{-16} \text{ dyn} & \text{for } r_0 = 1 \text{ cm} \\ 1 \text{ dyn} & \text{for } r_0 \simeq 1.5 \text{ \AA}; \end{cases} \quad (1.2)$$

¹ Since the force is measured in dyn = g cm s⁻² (1 dyn is equivalent to the force exerted by 1.0197 mg on its supporting surface), it is convenient to express the mass in Ws³cm⁻² with 1 Ws³cm⁻² = 10⁻⁷ g.

e is the elementary charge² ($= 1.6022 \times 10^{-19} \text{As}$). This force³ can be related to an electric field, F , via⁴

$$\mathcal{F} = eF; \quad (1.4)$$

hence one has

$$F = \frac{e}{4\pi\epsilon_0 r_0^2} \quad (1.5)$$

as the (constant) field on the intersecting line between the two point charges at distance r_0 between these charges.

1.1.1 The Poisson Equation

When applying *Gauss' law*, we can relate a region containing many charged particles (i.e., a space-charge region, neglecting the microscopic position of each individual particle), with $\varrho = ne$, to the field on a closed surface (of any shape) surrounding this space charge, and one obtains:

$$\oint \mathbf{F} d\mathbf{S} = \int \frac{\varrho}{\epsilon_0} d\mathcal{V} \quad (1.6)$$

where \mathcal{V} is the volume containing the space charge ne with n the density of charged particles, and $d\mathbf{S}$ is an element of the enclosing surface. For a sphere of the radius r_0 one can easily solve the closed surface integral $\oint d\mathbf{S} = 4\pi r_0^2$; hence the field normal to such a sphere at its surface is

$$F = \frac{\varrho \mathcal{V}}{4\pi\epsilon_0 r_0^2} = 1.44 \times 10^{-7} \frac{n (\text{cm}^{-3})}{r_0^2 (\text{cm}^2)} \left(\frac{\text{V}}{\text{cm}} \right) \quad (1.7)$$

which, for a sphere of 1 cm radius results is a field⁵ of $\simeq 1.44 \times 10^{-7} n \text{ V cm}^{-1}$.

The electric field is a vector that points from a positive to a negative charge, i.e., it points inward, normal to the surface of this sphere when its charge is negative. It decreases with increasing distance from the center of the sphere $\propto 1/r^2$. An *electrostatic potential difference* $\psi_{1,2}$, which describes

² The charge of an electron is $(-e)$.

³ It is interesting to recognize that the electrostatic force between two ions at a distance of 1.5 \AA is $\approx 1 \text{ dyn}$, i.e., on an order of magnitude that is well within the means of macroscopic sensors. This permits one to manipulate single atoms in an atomic force microscope.

⁴ The correct way to introduce the field-force relation is via a test charge in the limit of zero charge:

$$\mathbf{F} = \lim_{e \rightarrow 0} \vec{\mathcal{F}}/e. \quad (1.3)$$

⁵ It should be recognized that these fields are exceedingly large for uncompensated charges. For instance, when charging a sphere of 1 cm radius with only 10^{13} cm^{-3} electrons, one approaches already breakdown fields of the best insulators (a few times 10^6 V cm^{-1}).

the work required to move a positive test charge in this electric field from a position r_1 to r_2 is defined as

$$\psi_{1,2} = - \int_{r_1}^{r_2} F dr. \quad (1.8)$$

Since this work is defined to be negative when a positive test charge moves in direction of the field, 1.8 requires the $(-)$ sign for $r_2 > r_1$.

When an electron is moved from $r_2 = \infty$ to r_1 , one obtains the *absolute electrostatic electron potential*, which for the above given example is

$$\psi_n = - \int_{r_1}^{\infty} \frac{\rho \mathcal{V}}{4\pi\epsilon_0 r^2} dr = + \frac{\rho \mathcal{V}}{4\pi\epsilon_0 r_1}, \quad (1.9)$$

or, for a sphere of 1 cm radius, is $\psi \simeq 0.1 \mu\text{V}$ for every excess electron on the sphere.

In general one has

$$\oint \mathbf{F} d\mathbf{S} = \int \text{div } \mathbf{F} d\mathcal{V} = \int \frac{\rho}{\epsilon_0} d\mathcal{V}, \quad (1.10)$$

or,

$$\text{div } \mathbf{F} = \frac{\rho}{\epsilon_0}, \quad (1.11)$$

which is referred to as the *Poisson equation*. The relation between electric field and electrostatic potential can be written in general form as

$$\mathbf{F} = -\mathbf{grad}\psi = -\nabla\psi; \quad (1.12)$$

hence, Poisson's equation is often also given as

$$\text{div } \mathbf{grad}\psi = \nabla^2\psi = -\frac{\rho}{\epsilon_0}. \quad (1.13)$$

This equation holds when the distance r to a probing charge is sufficiently large compared to the distance between individual charges of the space-charge ensemble, so that a homogeneous, smeared-out collective of charges acts on the probing charge. The *granular texture* of the space charge can then be neglected.⁶

⁶ Modern devices become progressively smaller and represent typically a volume on the order of 10^{-4} cm in diameter. With a carrier density of 10^{16} cm^{-3} they contain a total of only 10^4 carriers in the bulk. In addition, the actual space-charge region has only a typical thickness of 10^{-5} cm and therefore contains less than 1,000 charged defects with an average distance between these charges of 1/30 of the device dimension. Statistical fluctuations ($\propto \sqrt{N}/N$) then become large. For smaller device dimensions, or lower space-charge densities, the granular texture of the charges can no longer be neglected. Here the continuum model is expected to approach its limits, and must be replaced by an atomistic picture, the carrier transport by a ballistic rather than diffuse transport.

In a semiconductor or insulator the force between two charges is reduced because of the *shielding influence* of the atoms between these charges. Such a shielding is described by the dielectric constant ε (more precisely by the static dielectric constant ε_{st} here):

$$\mathcal{F} = \frac{e^2}{4\pi\varepsilon\varepsilon_0 r^2}; \quad (1.14)$$

hence, the relation between field and space charge within a semiconductor is given by

$$\boxed{\operatorname{div} \mathbf{F} = \frac{\rho}{\varepsilon\varepsilon_0}}, \quad (1.15)$$

and between electrostatic potential and space charge by

$$\boxed{\nabla^2 \psi = -\frac{\rho}{\varepsilon\varepsilon_0}}. \quad (1.16)$$

In the following chapters we will only use one relevant space coordinate between these charges. The relationship between space charge and field is then given by the one-dimensional Poisson equation

$$\boxed{\frac{dF}{dx} = \frac{\rho}{\varepsilon\varepsilon_0}}. \quad (1.17)$$

Such a field distribution determines the electrostatic potential distribution for electrons via

$$\boxed{\frac{d\psi(x)}{dx} = -[F(x) - F(x=0)] = -\int_0^x \frac{\rho(\xi)}{\varepsilon\varepsilon_0} d\xi}, \quad (1.18)$$

with

$$\boxed{\psi(x) = \int_{d_1}^x F(\xi) d\xi}. \quad (1.19)$$

and for $\xi = d_1$, the corresponding $\psi(d_1)$ serves as reference point for the electrostatic potential.

In summary, we have shown that space-charge regions result in field inhomogeneities. The importance of such field inhomogeneities lies in their ability to influence the current through a semiconductor. With the ability to change space charges by changing a bias, as we will see later, they provide the basis for designing semiconducting devices.

Since a wide variety of space-charge distributions are found in semiconductors, many of which are of technical interest, we will first enumerate some of the basic types of these distributions and start with a catalogue of the interrelationships of various given $\rho(x)$, resulting in corresponding distributions of electric field $F(x)$ and electrostatic potential $\psi(x)$.

Because of the common practice to plot the distribution of the band edges for devices, we will follow this habit throughout the following sections. The band edge follows the electron potential $\psi_n(x)$ and this relates to the electrostatic potential as

$$E_c(x) = e\psi_n(x) + c = -e\psi(x) + \text{const.} \quad (1.20)$$

1.2 Fixed Space-Charge Distributions

In the examples given in this section, the *space-charge profiles* are arbitrarily introduced as fixed, explicit functions of the independent coordinate (x). The space charge can be kept constant in an insulator that does not contain free carriers. Here all charges are assumed to be trapped in now charged lattice defects.

1.2.1 Sinusoidal Continuous Space-Charge Distribution

A simple sinusoidal space-charge double layer can be described by

$$\varrho(x) = \begin{cases} ea \sin[2\pi x/d] & \text{for } -d/2 \leq x \leq d/2 \\ 0 & \text{elsewhere} \end{cases} \quad (1.21)$$

with $d = d_1 + d_2$ the width of the space charge layer; d_1 and d_2 are the widths of the negative and positive regions of the space charge double layer (here, $d_1 = d_2$). The space charge profile is shown in Fig. 1.1a.

The corresponding field distribution is obtained by integration of (1.21), and assuming $F(x = \pm\infty) = 0$ as boundary conditions:

$$F(x) = \begin{cases} -(ead) \cos[2\pi x/d] & \text{for } -d/2 \leq x \leq d/2 \\ 0 & \text{elsewhere;} \end{cases} \quad (1.22)$$

it is shown in Fig. 1.1b, and presents a negative field with a symmetrical peak; its maximum value lies at the position where the space charge changes its sign. The maximum field increases with increasing space-charge density ea and width d .

The corresponding electron energy (band edge) distribution is obtained by a second integration of 1.21, yielding with an assumed $E_c(\infty) = 0$ as boundary condition:

$$E_c(x) = \begin{cases} e^2 ad^2 / (4\varepsilon\varepsilon_0) & \text{for } x < -d/2 \\ -e^2 ad^2 \sin[2\pi x/d] / (4\varepsilon\varepsilon_0) & \text{for } -d/2 \leq x \leq d/2 \\ 0 & \text{for } x > d/2, \end{cases} \quad (1.23)$$

that is, a band edge step down of height $ead^2/(4\varepsilon\varepsilon_0)$, as shown in Fig. 1.1c.

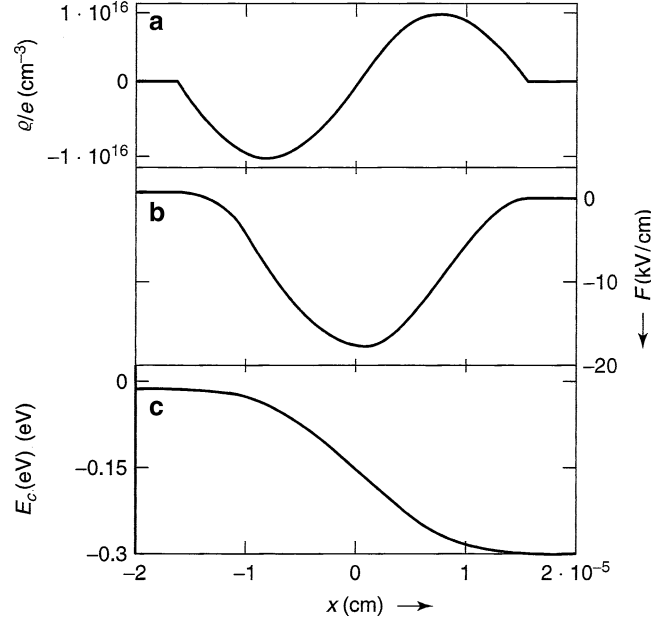


Fig. 1.1. Sinusoidal space charge, and resulting electric field and electron energy distributions. Computed for a maximum charge density, $a = 10^{16} \text{ cm}^{-3}$, a width $d = 3 \cdot 10^{-5} \text{ cm}$, and for a relative dielectric constant, $\varepsilon = 10$

Such behavior is typical: a **space-charge double layer** produces a *field spike* and a *band edge step*. For a $(-+)$ sequence of the space charge with increasing x (from left to right), the step is downward and the field spike is negative. The reversed space charge sequence $(+-)$ produces a positive field spike and a band edge step upward as shown in Fig. 1.2.

1.2.2 Abruptly Changing Space-Charge Distribution

All distributions of F and ψ are smooth when caused by the integration of a smooth space-charge distribution. As will be shown in Sect. 2.1, however, the charge distributions change abruptly from one sign to the other in many solids. A sinusoidal distribution with an abrupt change at $x = 0$ is therefore presented as an example in Fig. 1.3, curve set a:

$$\varrho = \begin{cases} 0 & \text{for } x < -d/2 \\ -ea \cos\left(\frac{2\pi x}{d}\right) & \text{for } -d/2 \leq x < 0 \\ ea \cos\left(\frac{2\pi x}{d}\right) & \text{for } 0 \leq x < d/2 \\ 0 & \text{for } d/2 \leq bx. \end{cases} \quad (1.24)$$

As a result, the field distribution is now given by a triangle and has a sharp peak (i.e., an abrupt change in slope) at $x = 0$ with equal values of

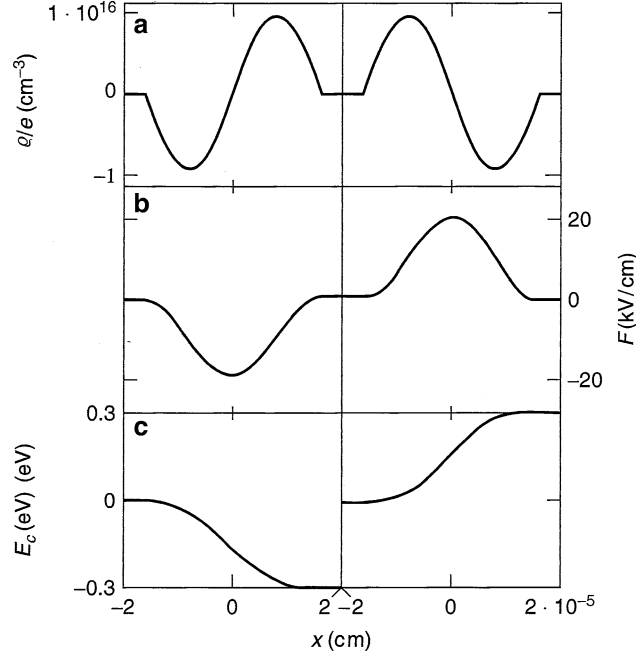


Fig. 1.2. Field extrema and band edge step signs depending on space-charge double layer sequence (computed as in Fig. 1.1)

the slope on either side. However, the potential distribution is still a smooth distribution and its shape is rather similar to the one produced by a smooth rather than abrupt change of the space charge.

Another often observed form of the space-charge distribution can be approximated by two step-functions:

$$\varrho = \begin{cases} 0 & \text{for } x < -d/2 \\ -ea & \text{for } -d/2 \leq x < 0 \\ ea & \text{for } 0 \leq x < d/2 \\ 0 & \text{for } d/2 \leq x \end{cases} \quad (1.25)$$

We assume again $d_1 = d_2$ for a symmetrical distribution, as shown in Fig. 1.3a, curve b. Here the value of the field increases linearly in the range of constant space-charge according to

$$F(x) = F_c - \frac{ea}{\varepsilon\varepsilon_o}x \quad \text{for } -d/2 \leq x < 0 \quad (1.26)$$

$$F(x) = F_c + \frac{ea}{\varepsilon\varepsilon_o}x \quad \text{for } 0 \leq x < d/2 \quad (1.27)$$

with the maximum value of the field F_c given by

$$F_c = -\frac{ead_1}{\varepsilon\varepsilon_o}, \quad (1.28)$$

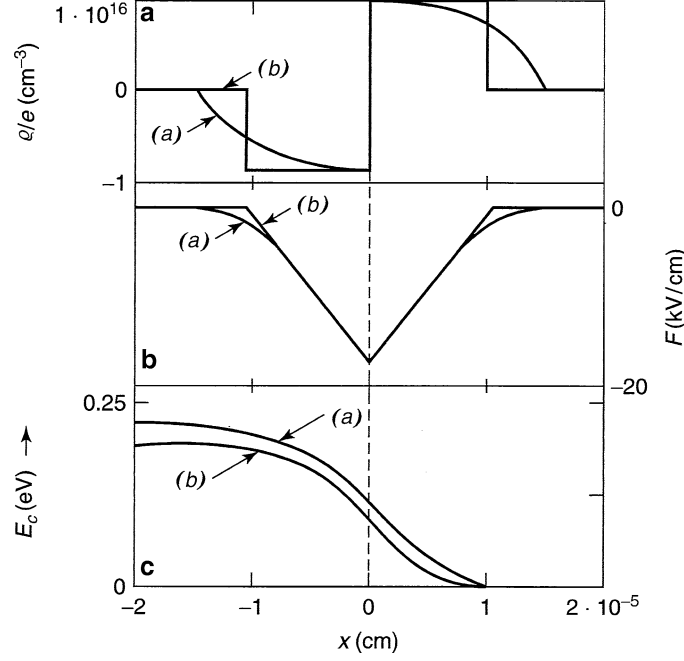


Fig. 1.3. (a) Space charge with an abrupt change of sign, resulting in corresponding (b) field and (c) band edge distributions: shown for (a) sinusoidal; and (b) step-like space charge distribution

shown in Fig. 1.3b, curve b. The band edge potential distribution, obtained by integration of (1.28) [using $E_c(x = \infty) = 0$ as boundary condition], changes parabolical:

$$E_c(x) = \begin{cases} \frac{e^2 a d_1^2}{\varepsilon \varepsilon_o} & \text{for } x < -d_1 \\ \frac{e^2 a d_1^2}{\varepsilon \varepsilon_o} + F_c x - \frac{e a}{2 \varepsilon \varepsilon_o} x^2 & \text{for } -d_1 \leq x < 0 \\ \frac{e^2 a d_2^2}{\varepsilon \varepsilon_o} + F_c x + \frac{e a}{2 \varepsilon \varepsilon_o} x^2 & \text{for } 0 \leq x < d_2 \\ 0 & \text{for } d_2 \leq x; \end{cases} \quad (1.29)$$

the total height of the band edge step for a symmetrical distribution with $d_1 = d_2$ is given by:

$$E_c(x = -d_1) - E_c(x = d_2) = \frac{e^2 a d_1^2}{4 \varepsilon \varepsilon_o}. \quad (1.30)$$

This simple shape evaluation of the field distribution within, and the potential drop across a step-like space-charge distribution is helpful in the evaluation of potential barriers and many junctions (see Sect. 3.1).

From (1.30) it is evident that a large potential drop (supporting a large applied voltage) can be obtained by either a large space-charge density ea or a wide space-charge width d . However, both quantities also cause a similar increase in the maximum field F_c (1.28), which may become too large and consequently could lead to an electrical breakdown of the device. An increase of the potential step *without* the increase in F_c can be obtained by inserting a neutral layer between the two space-charge regions, as will be discussed below.

1.2.3 Space-Charge Double Layer with Neutral Interlayer

Under certain conditions (e.g., via appropriate doping profiles or through field quenching, described in Sect. 3.3), the two space-charge regions can be separated by an extended range of vanishing space charges (see Fig. 1.4a). In this charge-neutral region the field remains constant (Fig. 1.4b), and the band edge step increases linearly (Fig. 1.4c). Large potential drops can be achieved by simply increasing the distance $(x_2 - x_1)$ between the two space-charge regions,

$$E_c^{(2)} - E_c^{(1)} = F_c \left[\frac{x_2 - x_1}{2} + \frac{d_1}{2} + \frac{d_2}{2} \right], \quad (1.31)$$

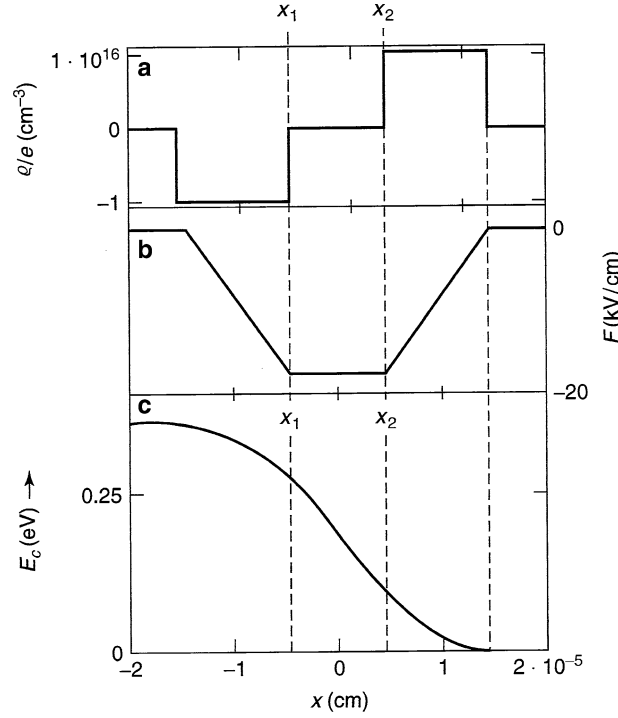


Fig. 1.4. (a) Step-like space-charge double layer with a neutral interlayer, resulting (b) a field distribution with constant center region and (c) a band edge change with a linear range in the middle distributions

d_1 and d_2 are the widths of each of the space-charge regions (see Sect. 3.3.3.1). The maximum field remains the same (for $d_1 = d_2 = d$) as given in (1.28):

$$F_c = -\frac{ead}{\varepsilon\varepsilon_o}. \quad (1.32)$$

This is an important means to increase the reverse blocking voltage of certain semiconducting devices.

1.2.4 Asymmetric Space Charge Double Layer

In all of the previous examples, a symmetrical charge double layer was assumed. With an asymmetrical space charge profile, the resulting field spike also becomes asymmetric and the band edge distribution becomes skewed (see Fig. 1.5, curve set a.)

In cases of highly asymmetrical profiles, the contribution of the high density part of the space-charge double layer can be neglected with respect to the band edge drop, as seen in Fig. 1.5, curve set b. In the region with $a = 10^{15} \text{ cm}^{-3}$, this band edge drop is 0.24 V; in the adjacent region with $a = 2 \cdot 10^{16} \text{ cm}^{-3}$, the additional band edge drop is only 1% of that and is barely visible in Fig. 1.5c, curve set b.

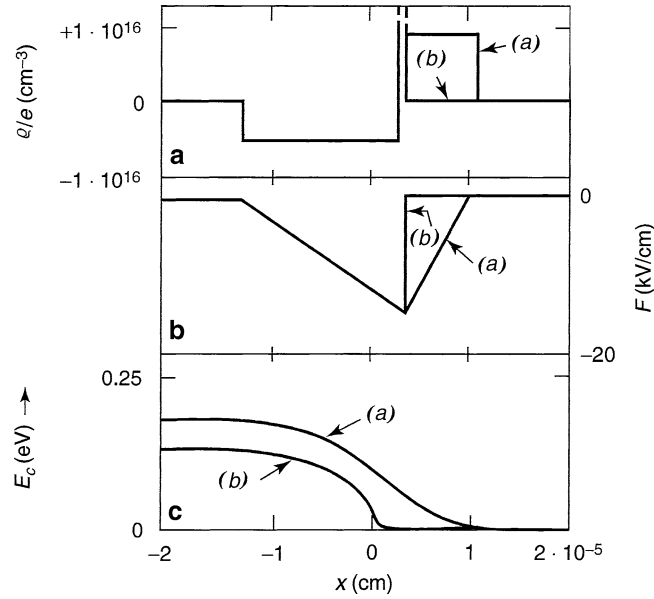


Fig. 1.5. (a) Asymmetric space-charge double layer and resulting (b) field and (c) band edge distributions with minor (a) and major (b) asymmetry, the latter results in a steeper change of the band edge distribution

In actual semiconductor junctions the doping of p - and n -type parts of the junction is usually asymmetric and the resulting space charge profile is similar to such highly asymmetrical double layers. The results shown in Fig. 1.5, curve set b, with resulting field and band edge distributions in the low charge density region *only*, are often used as a reasonable approximation to describe asymmetrical junctions.

1.2.5 Single Space-Charge Layer

In all previous examples we have assumed total charge neutrality within the given solid, i.e.,

$$\int_{-l_1}^{l_2} \varrho(x) dx = 0,$$

with l_1 and l_2 as the distance from the space-charge interface to the left or right semiconductor boundary (e.g., to its electrodes). If this neutrality condition is not fulfilled within one solid (e.g., some of the compensating charges of a semiconductor are located on the surface of the adjacent metal electrode), then the *effective* (net) *space charge* can be represented by a single layer within the bulk of the semiconductor.

Such a single space charge layer (Fig. 1.6a) causes a field-ramp as shown in Fig. 1.6b. Depending on the distance of this layer from the metal electrode

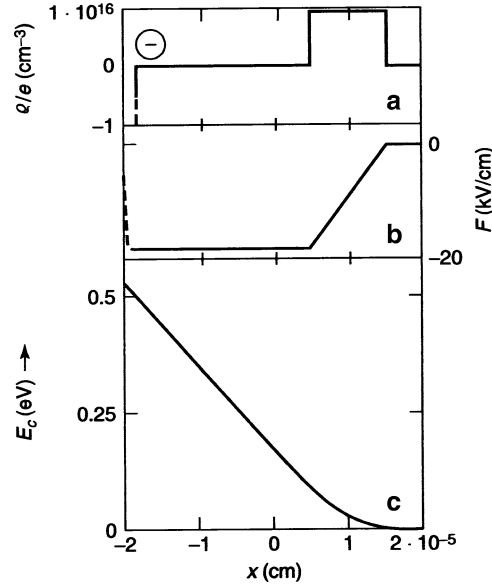


Fig. 1.6. (a) Single space-charge layer in the bulk with corresponding surface charge on the left electrode and resulting in a (b) field ramp and a (c) linear band edge slope in the field ramp region

where the compensating charges⁷ are located, the band edge drop increases in a manner similar to the example of an ordinary double layer with charge separations (1.31). In other words, the band edge increases parabolical (to the left) in the region of the field-ramp and then linearly in the adjacent space charge-free region toward the (left) electrode as shown in Fig. 1.6c. The field collapses at the surface of the left electrode due to the fact that it is a surface charge rather than a distributed space charge which would result in a more gradual decrease of $F(x)$. This collapse is indicated by the dashed line in Fig. 1.6b.

For reasons of maintaining a constant field in the homogeneous part of an actual semiconductor, a corresponding space charge separation with net charges sitting on both electrodes, is always present for nonvanishing net currents (see Sect. 2.1.1).

1.2.6 Space-Charge Double Layer, Nonvanishing Net Charge

We now extend the previous example to a nonsymmetrical double layer with a remaining net charge. The net charge is compensated by surface charges on the two electrodes. We assume that these surface charges are different in the two electrodes, resulting in a field distribution as shown in Fig. 1.7.

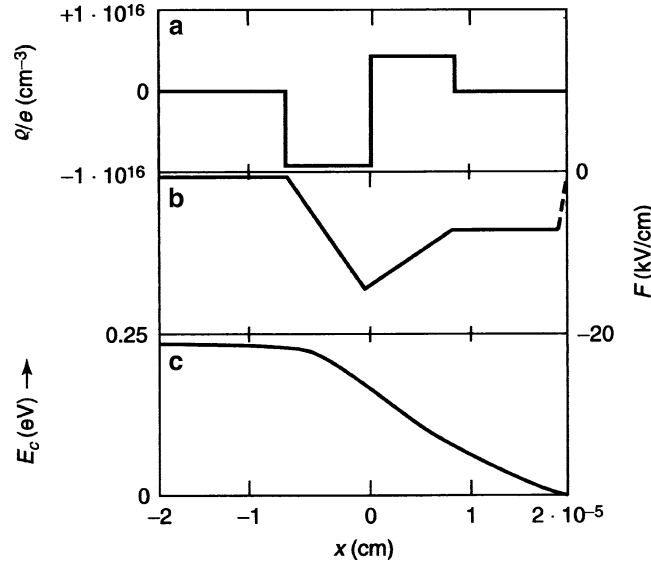


Fig. 1.7. (a) Asymmetrical space-charge double layer with asymmetric compensation on the two electrode surfaces and corresponding (b) field distribution showing the constant field range near the right electrode and (c) the band edge distribution with the linear range again corresponding to the constant field range distributions

⁷ It is assumed that such charges are at the surface of the left electrode in this example and indicated by the “-” sign in Fig. 1.6a.

Such a space-charge distribution is quite common for asymmetrical junctions with different conductivities in the adjacent bulk regions, hence causing different, but constant, fields in these regions when a bias voltage is applied. The major band edge drop usually occurs within the space-charge double layer, and the band edge drop⁸ in the adjacent bulk regions is considered a *series-resistance* perturbation.

Summary and Emphasis

Eight arbitrarily introduced space charge profiles are discussed as idealized examples to demonstrate the typical behavior that can be observed in various types of semiconductor devices. Though somewhat modified through the influence of mobile carriers, the principal trend remains the same and determines a number of device properties.

For instance, the field distribution in space charge double layers has usually a triangular shape with its maximum value at the double layer interface. The band edge shows a step.

If a diode is to be used at high bias conditions, a neutral interlayer between the positive and negative space-charge layers is necessary to achieve a sufficient voltage drop without running into breakdown fields.

Highly asymmetrical field and band edge distributions are common in asymmetrically doped *pn*-junctions. The potential drop in the highly doped (high space charge) region is usually negligible.

Series resistance effects, though undesired, are often a by-product of yet un-optimized solar cells or in some high-speed devices, e.g., in the base of bipolar transistors.

A clear understanding of the interrelation between space-charge distribution, the resulting field, and electron potential, corresponding to the band edge distribution assists in the task of designing devices with improved characteristics.

Exercise Problems

- 1.(e) Design an Si-diode with an *n*-type region, doped with 10^{16} cm^{-3} donors and a *p*-type region with 10^{17} cm^{-3} acceptors with an appropriate interlayer in which the field cannot exceed 10^5 V cm^{-1} and which can support a reverse bias of 10^3 V . Assume an ideal step-like space charge.
 - (a) How wide are the space charge layers in the *n*-type and *p*-type regions?
 - (b) How large are the voltage drops in both space charge regions?

⁸ Here enlarged for better clarity.

- (c) How thick must the neutral layer be?
- (d) How large is the voltage drop in the interlayer?
- 2.(r) List a number of semiconductor devices and classify them according to the examples given in this chapter. Explain the idealization in respect to the actual device.
- 3.(e) Relate the electrostatic potential distribution, electrostatic electron potential distribution, and band edge distribution for a given homo-junction; identify an external bias (applied voltage). Watch for proper sign, and energy vs. potential denotation.
- 4. Design an idealized space-charge distribution of your own that represents a typical semiconductor device. Insert typical space charge density values and layer thickness. Give field distribution and voltage drop quantitatively.
- 5. Derive the equivalence of the mass in units of $\text{Ws}^3\text{cm}^{-2}$.

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