Laboratory experiment

Determination of the Boltzmann constant employing VA-characteristics of a p-n junction

1.1 Tasks

1. Determine the Boltzmann constant by measuring the VA-characteristics of a p-n junction.

2. Determine the reverse bias saturation current of a p-n junction for three different temperatures.

3. In one graph, plot the VA-characteristics for all the (three) temperatures.

1.2 Note

On 20 May 2019, a new definition of the SI system of units came into force. Along with this new definition, some physical constants have been fixed, including the Boltzmann constant. The Boltzmann constant now has the value

$$k = 1.380\,649 \cdot 10^{-23}\,\text{J} \cdot \text{K}^{-1}.$$

This value is by definition exact, and the Boltzmann constant need not be measured. So the actual goal of this lab experiment is not to measure the value of the Boltzmann constant, but to test that the physical theory works, to learn some experimental techniques, and to try to process the measured data.

1.3 Theory

1.3.1 Electrons in electron clouds of isolated atoms

The state of an electron in the atomic electron cloud is completely determined by four quantum numbers n, l, m_l, and m_s. The principal quantum number n takes integer values of $1, 2, 3, \ldots$, and is mainly related to the energy of the electron[1]. The orbital quantum number l takes the values $0, 1, 2, \ldots, n-1$, it quantizes the magnitude of the orbital angular momentum of the electron. The

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[1] In a hydrogen atom or a hydrogen-like ion, the energy of the (single) electron depends only on this number, as n increases the negative energy of the electron increases (towards zero, the electron is bound in the atom, so the

magnetic quantum number m_l quantizes the projection of the orbital angular momentum of the electron onto any chosen axis and it takes the values $0, \pm 1, \pm 2, \ldots, \pm l$. The spin quantum number m_s takes the values $\pm 1/2$ and quantizes the projection of the internal angular momentum (spin) of the electron onto any chosen axis.

All states with the same value of n form the so-called shell, all states with the same value of n and l form the so-called sub-shell. Letters are often used instead of numbers to denote sub-shells: $s(l = 0)$, $p(l = 1)$, $d(l = 2)$, $f(l = 3)$, ... The energies of electrons in the shells of isolated atoms can only take discrete values. The energy of an electron in a sub-shell depends mainly on the quantum number n and to a lesser extent on the quantum number l. Within a given shell, the energy of the electron increases with increasing l.

According to Pauli exclusion principle, no two electrons in the same atom can have the same set of quantum number values. Hence, in one completely filled sub-shell there are $2(2l + 1)$ electrons (of different states) and in one filled shell there are $\sum_{l=0}^{n-1} 2(2l + 1) = 2n^2$ electrons. The electrons in the atom fill the individual shells and sub-shells so that the resulting energy of the atom is the smallest possible.

So, for example, neon has 10 electrons and the electron configuration of $1s^2, 2s^2, 2p^6$. This means that there are two electrons in the first $(n = 1)$ shell in the s sub-shell $(l = 0)$ (they differ in the spin quantum number), in the second shell $(n = 2)$ in the sub-shell s there are again two electrons differing in spin number and in the sub-shell p $(l = 1)$ there are 6 electrons (differing in the magnetic number $m_l = -1, 0, 1$ and the spin number $m_s = -1/2, 1/2$). Thus, all sub-shells are completely filled. Neon therefore has no weakly bound so-called valence electrons to form chemical bonds with other atoms and it is thus chemically neutral.

For example, sodium with 11 electrons has the electron configuration of $1s^2\, 2s^2\, 2p^6\, 3s^1$, which means that 10 electrons fully occupy shells 1 and 2 and that there is only one electron in the third shell $(n = 3)$ in the s sub-shell. This valence electron is only very weakly bound to the atom, and therefore sodium easily reacts chemically with atoms that have an unoccupied state ("hole") that can be "filled" by this electron.
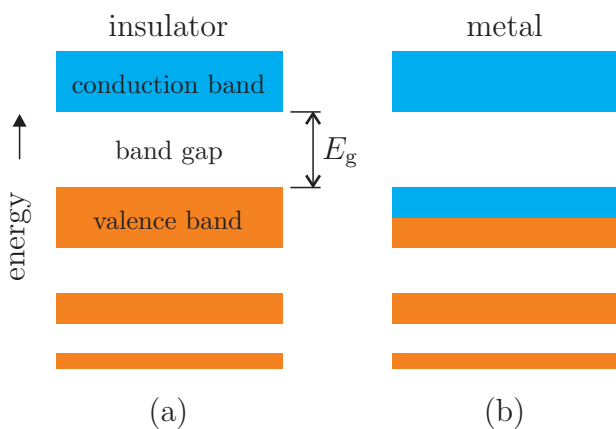

Figure 1.1: Energy bands of (a) insulators and (b) metals.

For example, chlorine with 17 electrons has the electron configuration of $1s^2, 2s^2, 2p^6, 3s^2, 3p^5$, which means that the $1s, 2s, 2p$ and $3s$ sub-shells are completely filled. Since the $3p$ sub-shell $(l = 1)$ can be filled with $2(2l + 1) = 6$ electrons, it is just one electron short of being fully occupied in chlorine. Thus, chlorine readily reacts chemically with atoms that have a valence electron that can fill this hole. For this reason, sodium chloride, for example, is a very stable compound.

1.3.2 Conduction of electric current in crystalline solids

In solids with a crystalline structure, the individual atoms are arranged in a periodic crystal lattice, with their mutual distances taking values on the order of 10^{-10} m. Because of these small distances

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higher its energy, the weaker it is bound). In atoms with multiple electrons the situation is more complex, since in addition to the attractive interaction with the nucleus, the electrons also interact repulsively with each other, which can result in partial shielding of the charge of the atomic nucleus and the resulting non-trivial dependence of the energy of the electron on the quantum numbers n and l.

(comparable to the dimensions of the individual isolated atoms), electron interactions also occur with neighboring atoms, resulting in the splitting of the individual discrete energy levels of the isolated atoms into as many levels as there are atoms in the crystal lattice.

Since the widths ΔE_i of the resulting *energy bands* take values on the order of electron-volts[2] and solids contain $N \approx 10^{23}$ atoms/cm^3, the individual energy levels within a bend are very tightly packed, there are very many of them and the bands can be considered continuous. Between these bands there are regions of energy that no electron can acquire. These regions are called the *band gaps.* For a solid to conduct an electric current, some electrons must move to higher energy levels.

Insulators

If the highest energy band containing electrons (the so-called *valence band*) is fully occupied, see Fig. 1.1a, the Pauli exclusion principle prevents electrons from moving to already occupied levels. Unoccupied energy levels are only available in the band above the band gap (the so-called *conduction band*), but to reach them the electron must overcome the energy E_g. If the band gap is wide enough, electrons have more or less no chance to overcome it and the material conducts almost no electric current. These materials are called *insulators*, (e.g., for diamond $E_g = 5.5\,\text{eV}$, the mean kinetic energy of thermal motion of the particle at room temperature $E_k \approx 0.04\,\text{eV}$).

Metals

It is characteristic of *metals* that the highest electron-occupied level is near the centre of the energy band, see Fig, 1.1b. If a voltage is applied to the metal, electrons from the highest occupied levels can gain some of the field energy to move to higher unoccupied energy levels. These so-called conduction electrons can then move freely, making metals good conductors of electric current.
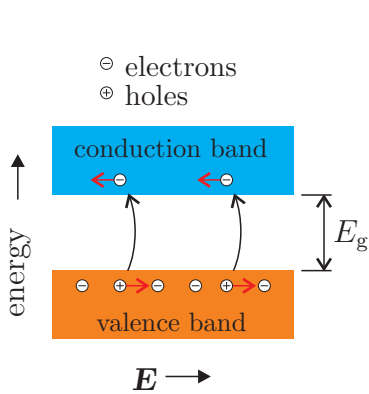
Semiconductors

Figure 1.2: Motion of electrons and holes in electric field $\boldsymbol{E}$.

So-called *semiconductors* have a similar band structure as insulators, see Fig. 1.1a, but in the case of semiconductors the band gap between the valence and conduction band is much narrower. For example, for silicon $E_g = 1.1\,\text{eV}$. Thus, for silicon (unlike diamond), even at room temperature, electrons can jump into the conduction band due to thermal agitation[3]. After these electrons, vacant energy states remain in the valence band–the so-called *holes.*

If we create in a semiconductor an electric field $\boldsymbol{E}$, see Fig. 1.2, electrons tend to move in the direction opposite to it[4]. Electrons in the conduction band can move freely due to the large number of unoccupied states, while electrons in the valence band can only fill unoccupied states, i.e., the holes. By this mechanism the holes drift in the direction of the electric field, their motion appears as that of positively-charged particles. Thus, in semiconductors, in addition to the electron conductivity, the hole conductivity is equally important.

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[2]One electron-volt ($1\,\text{eV}$) is the energy gained by an electron in a potential difference of one volt. Thus, $1\,\text{eV} = 1.602 \times 10^{-19}$ J.

[3]Resistivity of silicon is about $10^{11} \times$ higher than the one of copper at room temperature because the concentration of free charge carriers is about $10^{13} \times$ lower.

[4]For the electrostatic force acting on a particle with charge q, $\boldsymbol{F} = q\boldsymbol{E}$. Since the electron has a negative charge, the vectors $\boldsymbol{E}$ and $\boldsymbol{F}$ have opposite directions.
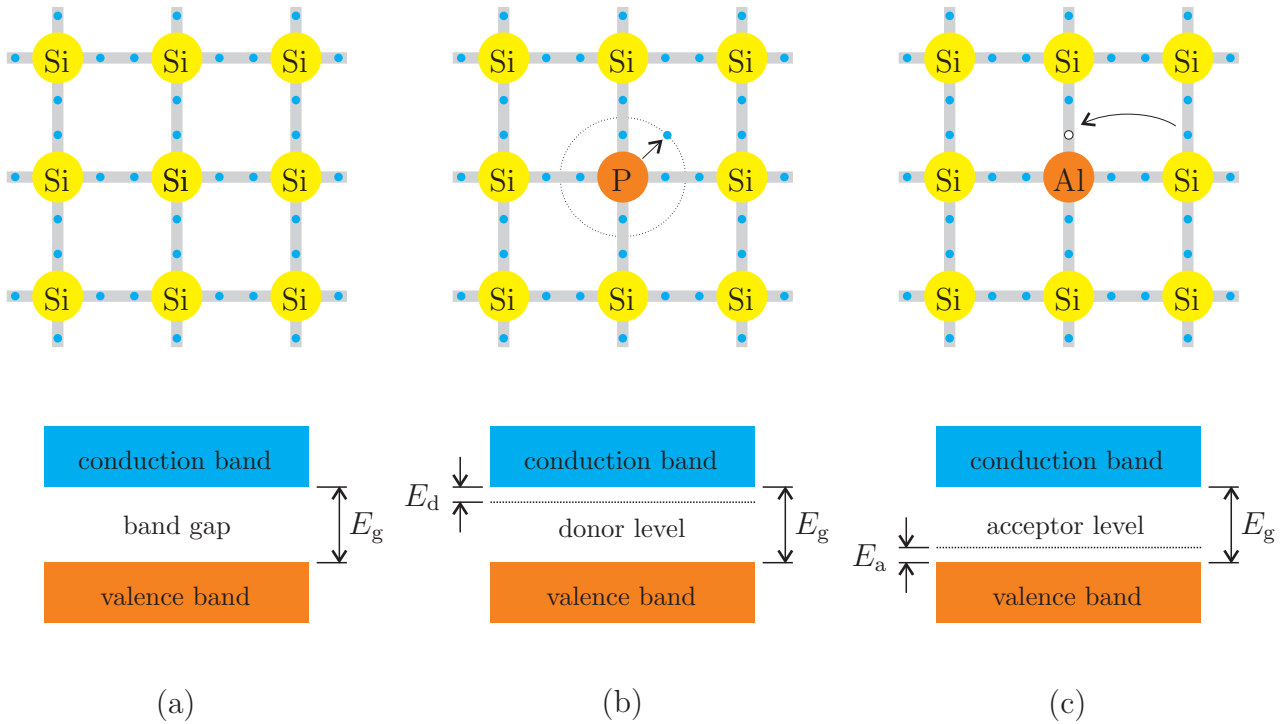
Figure 1.3: Two-dimensional model of crystal lattice and band structure of a) pure semiconductor, b) n-type semiconductor, and c) p-type semiconductor.

Doped semiconductors

The physical properties of semiconductors can be fundamentally altered by adding small amounts of impurity atoms – by so-called *doping*.

Figure 1.3a) shows a two-dimensional model of the crystal lattice of a typical semiconductor– silicon. The fourteen electrons in a silicon atom have the configuration $1s^2, 2s^2, 2p^6, 3s^2, 3p^2$. Each silicon atom contributes four weakly bound electrons from the $3s^2$ and $3p^2$ sub-shells to form a two-electron covalent bond[5] with each of their four neighbors. These electrons form the valence band in silicon. If one of these bonding electrons breaks off, it can travel through the crystal lattice (we say it has jumped the band gap to the conduction band).

If we replace a silicon atom in the crystal lattice with a phosphorus atom, see Fig. 1.3b, with 15 electrons in the configuration $1s^2\,2s^2\,2p^6\,3s^2\,3p^3$, only four of the five valence electrons (2 in the $3s$ sub-shell and 3 in the $3p$ sub-shell) participate in covalent bonds with neighboring silicon atoms. The remaining electron does not participate in the bonds and is only very weakly bound to the phosphorus atom. In the band diagram [Fig. 1.3b bottom] this electron occupies a localized state near the bottom of the conduction band, the energy E_d required for its transition to the conduction band is very small compared to the width of the band gap E_g ($E_d \approx 0.05\,\text{eV}$). We call the phosphorus atom the *donor* because it easily "donates" an electron into the conduction band. Due to the low value of E_d, even at room temperature, due to thermal agitation, almost all of the electrons supplied by the phosphorus atoms are in the conduction band, thus substantially increasing the number of conduction electrons. Semiconductors doped with donor atoms are called n-type semiconductors, where n-negative expresses that the number of negative charge carriers (electrons) in the conduction band greatly exceeds the number of positive charge carriers (holes) in the valence band. In a n-type semiconductor, electrons are *majority* carriers and holes are *minority* carriers.

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[5]In a covalent bond, two atoms share a pair of their electrons.

If we replace a silicon atom in the crystal lattice with, for example, an aluminum atom, see Fig. 1.3c, with 13 electrons in the configuration $1s^2\,2s^2\,2p^6\,3s^2\,3p^1$, only three valence electrons (2 from the $3s$ sub-shell and 1 from the $3p$ sub-shell) can participate in covalent bonds with neighboring silicon atoms. Thus, in one bond between aluminum and silicon there is a missing electron, i.e., a hole. By supplying only a small amount of energy, an electron can be pulled from an adjacent bond to fill this hole, but this creates a hole in the other bond and so it moves through the crystal lattice.
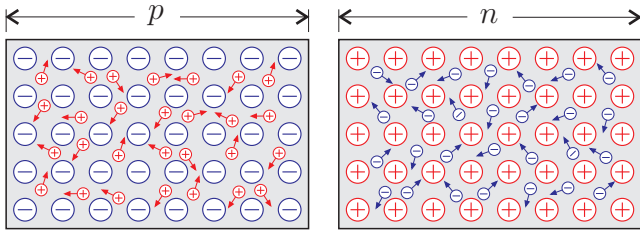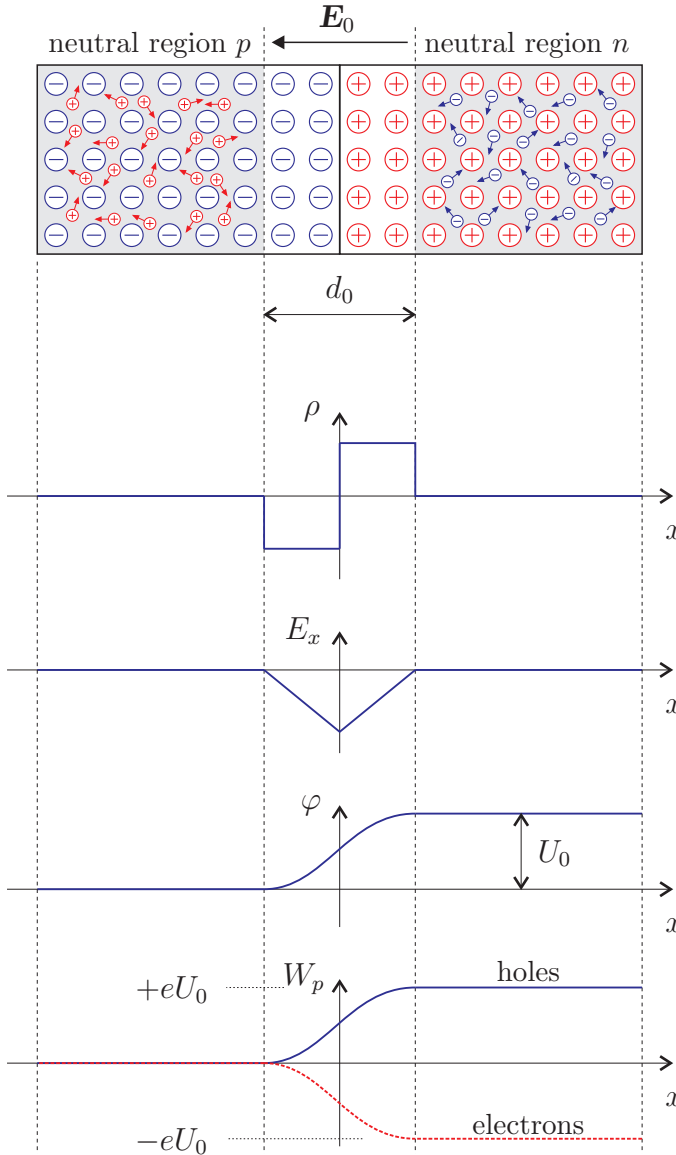
Figure 1.4: A p-n junction.

In the band diagram [Fig. 1.3c bottom], this electron occupies a localized state near the top of the valence band, the energy E_a required to move to this level from the valence band is very small compared to the width of the band gap E_g ($E_a \approx 0.05\,\text{eV}$). We call the aluminum atom an *acceptor* because it easily "accepts" an electron from the valence band. Due to the low value of E_a, even at room temperature, due to thermal agitation, almost all the acceptor levels of aluminum are occupied by atoms from the valence band, thus substantially increasing the number of holes in the valence band. Semiconductors doped with acceptor atoms are called p-type semiconductors, where p-positive indicates that the number of positive charge carriers (holes) in the valence band greatly exceeds the number of negative charge carriers (electrons) in the conduction band. In a p-type semiconductor, holes are *majority* carriers and electrons are *minority* carriers.

1.3.3   A p-n junction

A p-n junction is formed by a single crystal which is selectively doped with a p material in one part and a n material in the other, see Fig. 1.4. There is a high concentration of conduction electrons in the n-type semiconductor, while there is a high concentration of conduction holes in the p-type semiconductor. By combining the two semiconductors, see Fig. 1.4b, the concentration gradient near the junction plane results in the diffusion of conduction electrons from the n-region into the p-region and conduction holes from the p-region into the n-region. The diffusing electrons and holes near the junction plane merge (recombine) with each other, leaving positively charged immobile
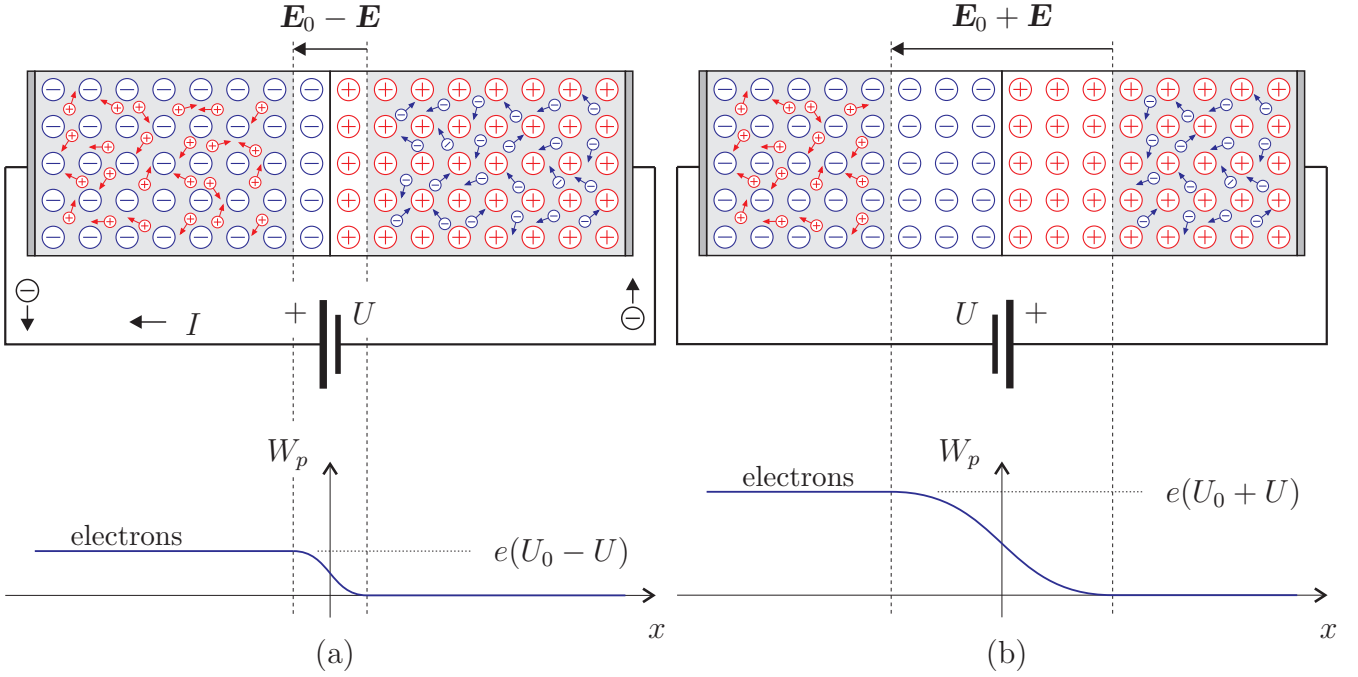
Figure 1.5: Forward- and reverse-biased p-n junction.

donor ions on the n-side and negatively charged immobile acceptor ions on the p-side.

This creates a region of space charge on each side of the junction plane. The volume density of the total charge ρ is schematically shown in Fig. 1.4c. This region is also called the *depletion zone* because it contains almost no mobile charge carriers, its width d_0 is depicted in Fig. 1.4b.

The space charge across the depletion zone gives rise to an electric field with intensity $\boldsymbol{E}_0$, see Fig. 1.4d and so-called *contact potential U_0*, see Fig. 1.4e. Due to the contact potential in the depletion zone, the potential energy of holes moving from the p-region to the n-region and electrons from the n-region to the p-region increases, see Fig. 1.4f, preventing further diffusion of the majority carriers across the junction plane.

For the minority carriers, i.e., holes in the n-region and electrons in the p-region, the situation is exactly the opposite, the contact potential drifts them across the junction plane. If no external voltage is applied to the p-n junction, a state of dynamic equilibrium establishes where the total current across the p-n junction generated by the motion of the majority and minority carriers is zero. Thus, the generation of the contact potential and the current of the minority carriers prevents unlimited charge transfer across the junction plane.

1.3.4 Forward- and reverse-biased p-n junction

Figure 1.5 a) shows a source of voltage U connected to a p-n junction such that the positive pole is connected to the p-region and the negative pole to the n-region. This makes the p-region more positive than before the source was connected and the n-region more negative, so electrons diffusing from the n-region to the p-region do not have to overcome the potential barrier of height eU_0, but only $e(U_0 - U)$. This greatly increases the probability of their passage through the junction plane. The same applies for holes diffusing from the p-region into the n-region. The external voltage also results in a narrowing of the depletion zone. Since it contains almost no mobile charge carriers and thus has a high resistivity, its narrowing results in a reduction of its electric resistance.

Electrons are added to the n-region from the negative terminal of the source, electrons leaving the p-region to the external circuit can be seen as a source of holes for the p-region, which means

that the semiconductor structure is constantly being replenished with majority charge carriers. The above results in a large current flowing through the p-n junction and we speak of the *forward-biased p-n* junction. The minority-carrier current is quite negligible compared to the majority-carrier current in this case, and the minority carriers are not replenished from the external source.

Figure 1.5 b) shows the opposite case, where the positive pole of the source is connected to the n-region and the negative pole to the p-region. Now the majority carriers diffusing across the junction plane must overcome a potential barrier of height $e(U_0 + U)$, which greatly reduces the probability of their passing through the junction plane. The electric resistance of the depletion zone increases due to its broadening. The current through the p-n junction is mainly due to the diffusion of minority charge carriers and is very small compared to the previous case, we speak of the *reverse-biased p-n* junction.

The above-mentioned properties of the p-n junction can be used to rectify alternating current, the corresponding electronic component is called a diode and is composed of just one p-n junction. The VA characteristics of an ideal diode reads

$$I = I_0 \left[\exp\left(\frac{eU}{kT}\right) - 1 \right], \tag{1.1}$$

where I_0 is the so-called reverse bias saturation current (it depends on the properties of the p-n junction and its temperature), e is the magnitude of the elementary charge, k is the Boltzmann constant, and T is the thermodynamic temperature (in kelvins).
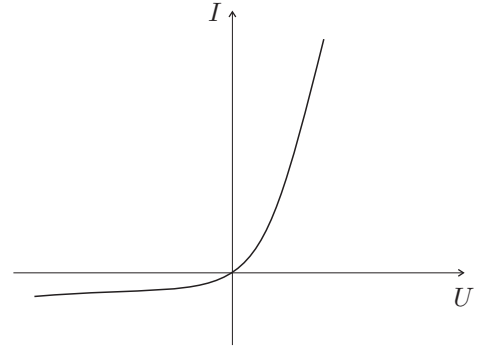

Figure 1.6: VA characteristics of a p-n junction.

1.4 Procedure

To measure the Boltzmann constant, we use the theoretical relation for the VA characteristics of the p-n junction (1.1). Since the measurements will be performed in the regime where $I \gg I_0$, we can simplify the relation (1.1) into the form

$$I = I_0 \exp\left(\frac{eU}{kT}\right). \tag{1.2}$$

Measured pairs of values (U_i, I_i), where $i = 1, \ldots, N$, are approximated employing the least squares method[6], by an exponential function

$$I = A\mathrm{e}^{\alpha U}, \tag{1.3}$$

the result of which are the coefficients A and α. Comparison of Eqs. (1.2) and (1.3) gives the relations for the determination of the sought quantities

$$I_0 = A, \qquad k = \frac{e}{\alpha T}.$$

The measurement of the VA characteristics of the p-n junction can be conducted in two ways:

1. VA characteristics measurements can be conducted directly on a diode. To minimize the measurement error, it is necessary to use the circuit as shown in Fig. 1.7.

   Moreover, it is necessary to use a voltmeter with a sufficiently large internal resistance to measure the voltage U on the diode, i.e., the smallest measured current through the diode I_{dmin} should be that $I_{\mathrm{dmin}} \gg I_{\mathrm{V}}$, where I_{V} is the current through the voltmeter.

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[6]For the calculations (and plotting graph) you can use the *Universal tool for plotting graphs* at *http://planck.fel.cvut.cz/praktikum/*.
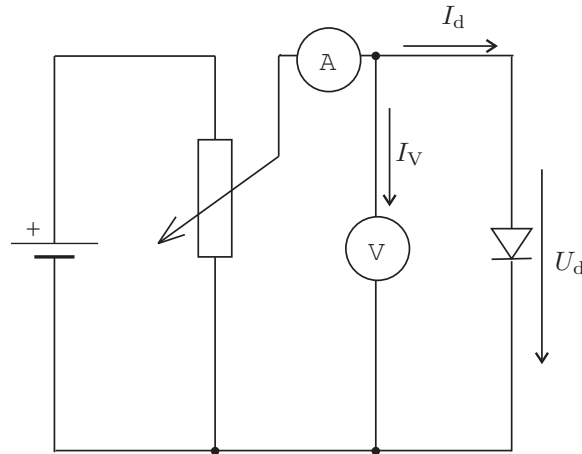
Figure 1.7: Principle circuit diagram for the p-n junction measurement employing a diode.
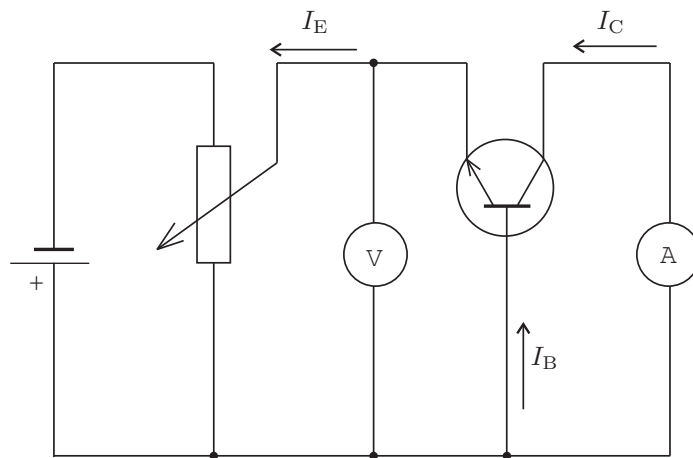

Figure 1.8: Principle circuit diagram for the p-n junction measurement employing a transistor.

2. Another possibility (**it is employed within this lab experiment**) to measure the VA characteristics of a p-n junction is to use a transistor in a common base connection, see Fig. 1.8.

   With a small voltage drop on the ammeter used, the voltage between the collector and base $U_{CB} \doteq 0$. Then the residual current $I_{CB} \doteq 0$ and for the collector current I_C it applies

   $$I_C = \frac{\beta_0}{\beta_0 + 1} I_E \; ,$$

   where β_0 is the amplification factor and I_E is the emitter current. If it applies $\beta_0 \gg 1$, then $I_C \doteq I_E$. Thus, the emitter current passes through the measured base-emitter p-n junction, but continues from the base region to the collector where it is measured. The ammeter is thus not connected in series with the measured p-n junction and does not affect the voltage measured at the p-n junction.

Based on the above text, the actual measurement can be conducted as follows:

1. Measurements are conducted for three different temperatures that are sufficiently far apart of each other. The selected temperatures of the p-n junction are maintained by the heat baths in which the measured p-n junction is immersed. For this purpose a Dewar flask (thermos) is
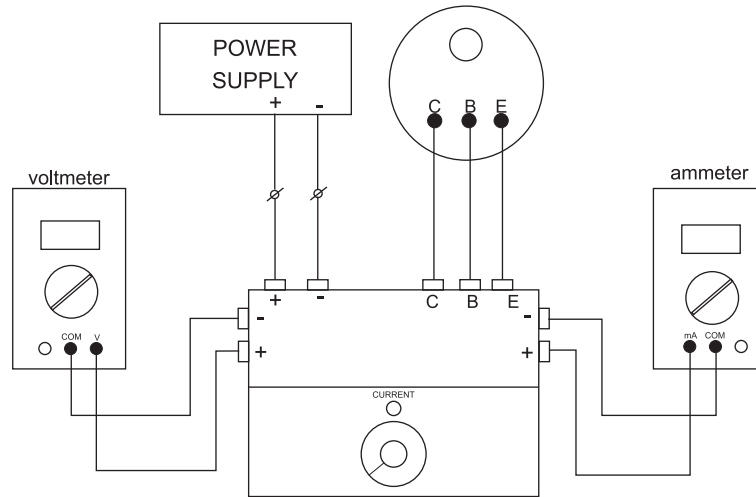
Figure 1.9: Experimental set-up.

used, filled with water up to the mark inside. Choose the different bath temperatures so that the difference between them is as large as possible, i.e., use cold, lukewarm and hot water. An electric kettle can also be used to obtain higher bath (water) temperatures, and the water temperature should not exceed 60°C.

2. Connect the measured p-n junction according to the appropriate scheme (Fig. 1.9) and immerse it in the heat bath.

3. After equalizing the temperature between the bath and the p-n junction, use a thermometer to read the bath temperature and start the actual measurement of the VA characteristics. At the end of the measurement, read the bath temperature again and use both the temperatures to determine the mean value. The measurements are conducted only in the forward-bias regime in the current range from approx. $0.5\,\mathrm{mA}$ to approx. $24\,\mathrm{mA}$.

4. Empty the Dewar flask after the measurement is completed.

5. Process the measured values using the least squares method (see above) and determine the Boltzmann constant k, the reverse bias saturation current I_0 and their uncertainties.

6. Repeat the measurement in the same way for the two other temperatures.

7. Plot the VA characteristics measured for all three temperatures in one graph.

1.5   References

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