

Derivation of the General Equation of State for a Doped Semiconductor. The Equation is Solved Concerning the Electron Concentration in the Conduction Band for Different Concentrations and Properties of Doping Substances

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Abstract

Original Research Article

The paper examines the state of a system consisting of a crystalline semiconductor doped with donor and acceptor impurities. The General Equation of State of the system is derived. Methods are proposed to solve the general equation for the concentration of electrons or holes in a semiconductor. The identity of the General Equations of State of semiconductors and aqueous solutions of electrolytes is discussed. An assumption is made about the practical application of the found relationships.

Keywords: Semiconductor, Silicon, Germanium, Electrons Concentration, Holes Concentrations, The General Equation of State.

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INTRODUCTION

The commonality of some properties of semiconductors and aqueous solutions of electrolytes has long been noted. For example, a pure crystalline semiconductor and pure water are not conductors of electric current, and the specific electrical conductivity of a doped semiconductor and an aqueous solution of the electrolyte increases with increasing temperature, in contrast to metallic conductors, where it decreases. An important commonality between crystalline semiconductors and water is that in semiconductors, the product of the electron and hole concentrations is the constant for a given semiconductor at a given temperature ($n \cdot p = \text{constant}$) (Electrons and Holes in Semiconductors 2020). The ionic product of water (K_w) is also a constant, and these constants are strongly temperature-dependent. From a mathematical point of view, the General Equation of State of aqueous solutions of electrolytes (Yefimov S. 2023) and the General Equation of State of a doped semiconductor, derived in this work, turned out to be completely identical. This identity encourages us to look for other physical commonalities between aqueous solutions and semiconductors. Here we consider the most general case of no full ionization of dopant at the semiconductor.

MATERIALS AND METHODS

The derivation of the General Equation of State is based on three expressions taken as axioms: 1) The expression for the ionization constant of an impurity in a semiconductor crystal, which is equivalent to the dissociation constant of an electrolyte in a solution, 2) the equation of electroneutrality, which states that the sum of positive charges in a solution (liquid or solid) is equal to the sum of negative charges, and 3) The product of the concentrations of positively and negatively charged charge carriers (electrons and holes) in a given semiconductor crystal is constant at a given temperature. We will call it the semiconductor constant, for example, the Silicon Constant (S). For the numerical calculations, the Microsoft EXCEL spreadsheet was used.

RESULTS AND DISCUSSION

Derivation of the Equation of State

The derivation of the equation of state consists of 7 stages: 1) The reaction scheme of the ionization process in a semiconductor; 2) An equation is written for the degree of ionization, which is an auxiliary variable; 3) An equation is written for the ionization constant; 4) The degree of ionization is expressed in terms of the ionization constant; 5) The equation of electrical neutrality is written; 6) All members of the electrical

neutrality equation are expressed in terms of known variables and coefficients; 7) The electrical neutrality equation thus obtained is converted into a normal polynomial.

We assume the system has a constant unit volume of 1L. For the convenience of deriving the equation, we introduce the following temporary abbreviations:

D^{+i} - a molar concentration of the ionized donor in the crystal.

Multi-step ionization process: $D \xrightarrow{-K_1} D^+ \xrightarrow{-K_2} D^{2+} \xrightarrow{-K_3} D^{3+}$.

$D, D^+, D^{2+},$ and D^{3+} are the molarity of the donor and ionized donors in the crystal. Ionization is not complete, and an equilibrium is established between the ionized and non-ionized donor. $K_1, K_2,$ and K_3 are ionization constants that we consider known. Let's introduce auxiliary variables $C_1, C_2,$ and C_3 - Ionization Degrees of the first, second, and third ionization stages.

Now let's write down the equations that will be needed to derive the general equation of state:

$A \rightarrow A^- + p^-$ an acceptor's ionization.

Let's write 3 lines of the equations of a donor's ionization, using the Ionization Degree definition and the Mass-Action law:

$D \rightleftharpoons D^+ + n; D^+ = D^* C_1, K_1 = n^* D^+ / (D - D^+), C_1 = K_1 / (K_1 + n), D^+ = D^* K_1 / (K_1 + n)$

$D^+ \rightleftharpoons D^{2+} + n; D^{2+} = D^{+*} C_2, K_2 = n^* D^{2+} / (D^+ - D^{2+}), C_2 = K_2 / (K_2 + n), D^{2+} = D^{+*} K_2 / (K_2 + n)$

$D^{2+} \rightleftharpoons D^{3+} + n; D^{3+} = D^{2+*} C_3, K_3 = n^* D^{3+} / (D^{2+} - D^{3+}), C_3 = K_3 / (K_3 + n), D^{3+} = D^{2+*} K_3 / (K_3 + n)$

Now rewrite the equation for ionized donors:

$D^+ = D^* K_1 / (K_1 + n)$

$D^{2+} = D^* K_2 K_1 / ((K_2 + n)(K_1 + n))$

$D^{3+} = D^* K_3 K_2 K_1 / ((K_3 + n)(K_2 + n)(K_1 + n))$

Now let's write down the Electroneutrality equation assuming complete ionization of the acceptor ($A=A^-$):

$D^+ + D^{2+} + D^{3+} + S/n = A + n.$ expanded equation:

$$D^* K_1 / (K_1 + n) + D^* K_2 K_1 / ((K_2 + n)(K_1 + n)) + D^* K_3 K_2 K_1 / ((K_3 + n)(K_2 + n)(K_1 + n)) + S/n = A + n. [**]$$

This is the equation of state of the system, it includes only known or given variables and constants: $A, D, K_1, K_2, K_3, S,$ and the desired value $n.$ We limited ourselves to the K_3 constant, but you can similarly write an equation for an n -step ionization donor ($n > 3$). Now let's convert the fractional notation $[**]$ to a linear one and group the terms:

$n^5 + a^* n^4 + b^* n^3 + c^* n^2 + d^* n + e = 0 [***].$ This is the normal form of the General Equation of State for a semiconductor doped with a stepwise ionizing donor and completely ionizing acceptor. The coefficients (a, b, c, d) are presented in Table 1.

It is easy to show, that if we put $K_3=0,$ then from the equation $[***]$ we get the equation for a two-stage ionizing donor, and if $K_3=0$ and $K_2=0,$ then we get the equation for a one-stage ionizing donor Table 1.

A mixture of several donors. The equation of state for a mixture of donors is derived in the same way as in the previous case. The equation contains the amount of each of the donors ($D_1, D_2, \dots D_n$), ionization constants (K), and the amount of acceptor (A). Let us derive the equation of state for a mixture of two donors, $D_1 (K_1, K_2)$ and $D_2 (K_3).$ Passing all the above steps of the derivation we take the equation of state:

$n^5 + a^* n^4 + b^* n^3 + c^* n^2 + d^* n + e = 0,$ the coefficients $a, b, c, d,$ and e are given in Table 1.

Note 1:

*The equation of state of a semiconductor doped with a stepwise ionizing acceptor and a fully ionizing donor is symmetrical to this $[***].$ The donor ionization constants are replaced by the acceptor ionization constants, D is replaced by A, A is replaced by $D,$ and n is replaced by p —the molarity of holes in the semiconductor.*

Using this method, equations of state can be derived for many systems and used to predict the behavior of semiconductors.

Table 1: Polynomial coefficients of the General Equation of State the semiconductor is doped with a donor and a fully ionizing acceptor

Max. degree.	The mix of two-stage ionizing donor $D_1(K_1, K_2)$ and one-stage ionizing donor. $D_2(K_3). n^5 + a^* n^4 + b^* n^3 + c^* n^2 + d^* n + e = 0$	Three-stage ionizing donor. $n^5 + a^* n^4 + b^* n^3 + c^* n^2 + d^* n + e = 0$	Two-stage ionizing donor. $n^4 + a^* n^3 + b^* n^2 + c^* n + d = 0$	One-stage ionizing donor $n^3 + a^* n^2 + b^* n + c = 0$	Completely ionizing donor. $n^2 + a^* n + b = 0$
n^5	1	1	0	0	0
n^4	$A + K_1 + K_2 + K_3$	$A + K_1 + K_2 + K_3$	1	0	0
n^3	$K_1 * K_2 + K_1 * K_3 + K_2 * K_3 + A * (K_1 + K_2 + K_3) - S - D_1 * K_1 - D_2 * K_3$	$K_1 * K_2 + K_1 * K_3 + K_2 * K_3 + A * (K_1 + K_2 + K_3) - S - D * K_1$	$A + K_1 + K_2$	1	0

n^2	$K1 \cdot K2 \cdot K3 + A \cdot (K1 \cdot K2 + K1 \cdot K3 + K2 \cdot K3) - S \cdot (K1 + K2 + K3) - D1 \cdot (2 \cdot K1 \cdot K2 + K1 \cdot K3) - D2 \cdot (K1 \cdot K3 + K2 \cdot K3)$	$K1 \cdot K2 \cdot K3 + A \cdot (K1 \cdot K2 + K1 \cdot K3 + K2 \cdot K3) - S \cdot (K1 + K2 + K3) - D \cdot (2 \cdot K1 \cdot K2 + K1 \cdot K3)$	$A \cdot (K1 + K2) + K1 \cdot K2 - S - D \cdot K1$	$A + K1$	1
n	$A \cdot K1 \cdot K2 \cdot K3 - S \cdot (K1 \cdot K2 + K1 \cdot K3 + K2 \cdot K3) - 2 \cdot D1 \cdot K1 \cdot K2 \cdot K3 - D2 \cdot K1 \cdot K2 \cdot K3$	$A \cdot K1 \cdot K2 \cdot K3 - S \cdot (K1 \cdot K2 + K1 \cdot K3 + K2 \cdot K3) - 3 \cdot D \cdot K1 \cdot K2 \cdot K3$	$A \cdot K1 \cdot K2 - S \cdot (K1 + K2) - 2 \cdot D \cdot K1 \cdot K2$	$A \cdot K1 - S - D \cdot K1$	$A - D$
n^0 (const.)	$-S \cdot K1 \cdot K2 \cdot K3$	$-S \cdot K1 \cdot K2 \cdot K3$	$-S \cdot K1 \cdot K2$	$-S \cdot K1$	$-S$

Let us add two important cases to our consideration.

It's not a completely ionizing acceptor. The equation of state will contain both the donor ionization constant K_n and the acceptor ionization constant K_p . The derivation of the equation is like the one above:

Let $K_n = K1$, $K_p = K2$

$C_n = K1 / (K1 + n)$

$C_p = K2 / (K2 + p) = K2 \cdot n / (K2 \cdot n + W)$

$D \cdot C_n + W/n = n + A \cdot C_p$ (equation of electrical neutrality)

$D \cdot K1 / (K1 + n) + W/n = n + A \cdot K2 \cdot h / (K2 \cdot n + W)$. After transformations, we get the equation of state in normal form: $n^4 + a \cdot n^3 + b \cdot n^2 + c \cdot n + d = 0$, where:

$a = A + K1 + S/K2$

$b = A \cdot K1 + S \cdot K1 / K2 - S - D \cdot K1$

$c = -(S \cdot K1 + D \cdot S \cdot K1 / K2 + S^2 / K2)$

$d = -K1 \cdot S^2 / K2$

A mixture of several donors. The equation of state for a mixture of donors is derived in the same way as above. The equation contains the amount of each of the donors ($D1, D2, \dots, Dn$), ionization constants (K), and the amount of acceptor (A). Let us derive the equation of state for a mixture of two donors, $D1$ ($K1, K2$) and $D2$ ($K3$). Passing all the above steps of the derivation we take the equation of state:

$n^5 + a \cdot n^4 + b \cdot n^3 + c \cdot n^2 + d \cdot n + e = 0$, the coefficients a , b , c , d , and e are in Table 1.

Solution of the Equations of State in Radicals

In the physics literature (Electrons and Holes in Semiconductors 2020), the concentration of charge carriers in a semiconductor is traditionally denoted in units of ($1/\text{cm}^3$). Chemists denote concentrations in moles (M), the relationship between the quantities is $1/\text{cm}^3 = 0.1666 \cdot 10^{-20} M$. This paper will follow chemical notations to compare the results obtained for semiconductors and aqueous solutions (Yefimov S. 2023). Now let's proceed directly to solving the problem

posed - determining the concentration of conduction electrons in an impurity semiconductor as a function of D and A , considering the parameters K and S or Ge at constant temperature and pressure: $n = f(A, D, s, k)_{T, P}$, $n = f(A, D, K_{Ge}, k)_{T, P}$.

Solving equations in radicals (Утешев А. 2022) will give us a formula with which we can plot the dependence of the concentration of electrons on the variables - D and A and parameters $K1, K2, K3, S, Ge$. Thanks to the work of Omar Khayyam (1048–1131), Niccolo Tartaglia (1500–1557), Gerolamo Cardano (1501–1576), Lodovico Ferrari (1522–1565), and other great mathematicians, we know how to find the roots of polynomials 2nd, 3rd, and 4th degree. Each equation of state has as many roots as its degree, but we are only interested in one real, positive root, and as we will show below, such a root exists. Let's formulate the Chemist's Theorem (Yefimov S. 2023): "The equation of state presented as a normal polynomial of the n -th degree with real coefficients has at least one real positive root if the free term of the polynomial is negative ($a_n < 0$)". This can be verified visually by moving the polynomial graph along the coordinate plane. In Table 1, the bottom row shows the free terms of the polynomials, all of which are negative, so the real positive root exists.

Completely Ionizing Donor and Acceptor

In the simplest case, both the donor and acceptor are completely ionized in the semiconductor. This case is described by the General Equation of State of the 2nd degree (Table 1.) The roots of the quadratic equation are found most easily:

$n = (D-A)/2 + \sqrt{d}$ (&), where $d = (D-A)^2/4 + S$ is discriminant of this quadratic equation. The curve's inflection point (Figure 1. b) corresponds to the equality of the concentrations of electrons and holes in the semiconductor, $n = \sqrt{S}$.

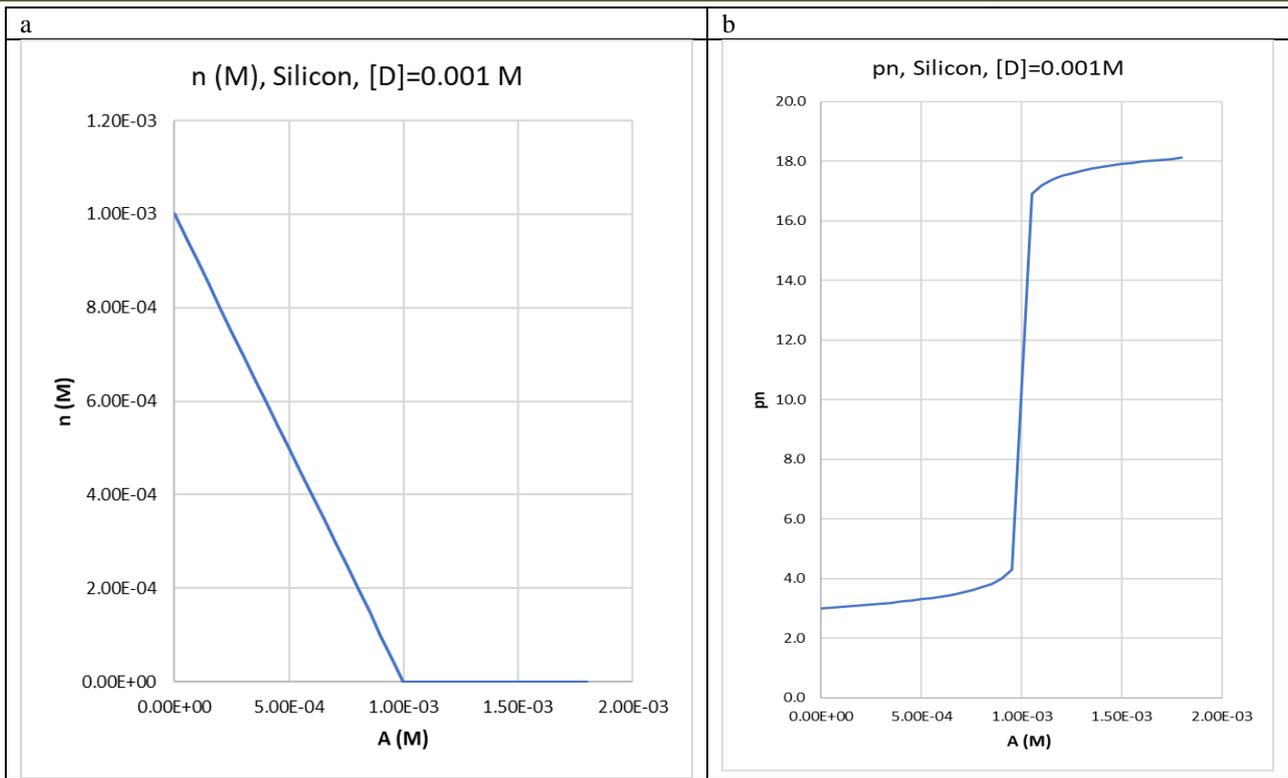


Figure 1 a, b: Dependence of the electron concentration (n) and (pn) on the change in the concentration of the acceptor impurity in the simplest case.

The donor is not completely ionized in one ionization stage with constant K1. This case is described by a 3rd-degree polynomial (Table 1). The formula finds the roots of the cubic equation:

$$n = y - a/3, \text{ where}$$

$$y = 2 \cdot \sqrt{-p/3} \cdot \cos(\varphi/3)$$

$$\varphi = \arccos(3 \cdot q \cdot \sqrt{-3/p} / (2 \cdot p))$$

$$p = b - a^2/3,$$

$$q = 2 \cdot a^3/27 - a \cdot b/3 + c$$

For details see Appendix #1.

The graph of the solution of this equation in the n-A-D coordinate system represents a surface and a line in n-A (Figure 2). The curve's inflection point (Figure 2. b) corresponds to the equality of the concentrations of electrons and holes in the semiconductor, $n = \sqrt{q}(S)$.

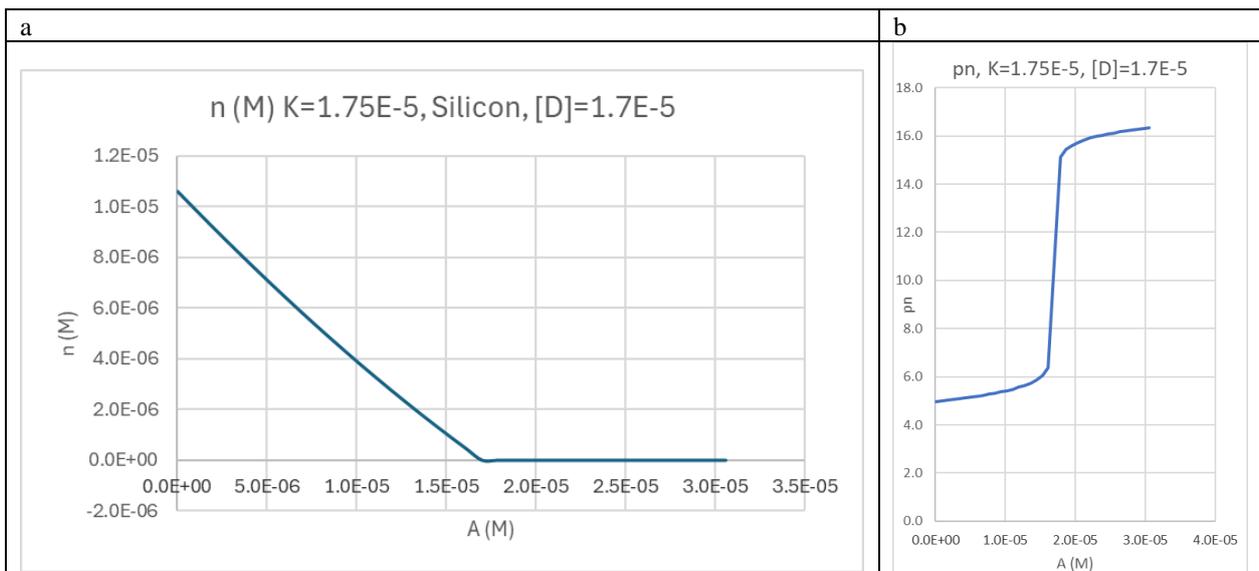


Figure 2 a, b: Dependence of the electron concentration (n) and (pn) on the change in acceptor concentration. Donor ionization occurs in one stage with the constant K1. The value of the constant is chosen arbitrarily for better clarity of the curve behavior.

The donor is not completely ionized. The ionization occurs in two stages with constants K1 and K2. This case is described by a 4th-degree polynomial (Table 1). To find the root, it is necessary to take several steps and make several changes to variables (Утешев А. 2022). The equation gives the root (n):

$$\begin{aligned}
 n &= x - a/4 \\
 x &= K/2 + \sqrt{D} \\
 D &= K^2/4 - (t/2 - L) \\
 K &= \sqrt{t - p} \\
 L &= q/(2 * K) \\
 t &= y - \alpha/3 \\
 y &= 2 * (-\Pi/3)^{1/2} * \cos(\varphi/3) \\
 \varphi &= \arccos(3 * Q * (-3/\Pi)^{1/2} / (2 * \Pi)) \\
 \Pi &= \beta - \alpha^2/3 \\
 Q &= 2 * \alpha^3/27 + \varepsilon - \alpha * \beta/3 \\
 \alpha &= -p \\
 \beta &= -4 * r \\
 \varepsilon &= 4 * p * r - q^2 \\
 p &= b - 3 * a^2/8 \\
 q &= a^3/8 - b * a/2 + c \\
 r &= d - c * a/4 + b * a^2/16 - 3 * a^4/256
 \end{aligned}$$

See Appendix#2 for details.

The dependence $n=f(A, D, K_1, K_2)$ based on the root of the polynomial is presented in Figure 3.

Fortunately, the terms A and D are presented in the General Equation of State in the first degree:

$$n^4 + (A + K_1 + K_2) * n^3 + (A * (K_1 + K_2) + K_1 * K_2 - S - D * K_1) * n^2 + (A * K_1 * K_2 - S * (K_1 + K_2) - 2 * D * K_1 * K_2) * n - S * K_1 * K_2 = 0,$$

so, we can express A as function of n and D:

$$A = [(S * K_1 * K_2 - n^4 - n^3 * (K_1 + K_2) - n^2 * (K_1 * K_2 - S - D * K_1) + n * (K_1 * S + K_2 * S + 2 * D * K_1 * K_2)] / (n^3 + n^2 * (K_1 + K_2) + n * K_1 * K_2)$$

We can plot dependence $A=f(n)$ and $A=f(pn)$ using this formula. Figure 3(b) shows the dependence of pn on A obtained by solving the General Equation of State (solid line) and using the formula &&& (symbols (pn2)). Both lines coincide. The formula &&& is useful for finding the inflection points of the curve (Yefimov S. 2023)

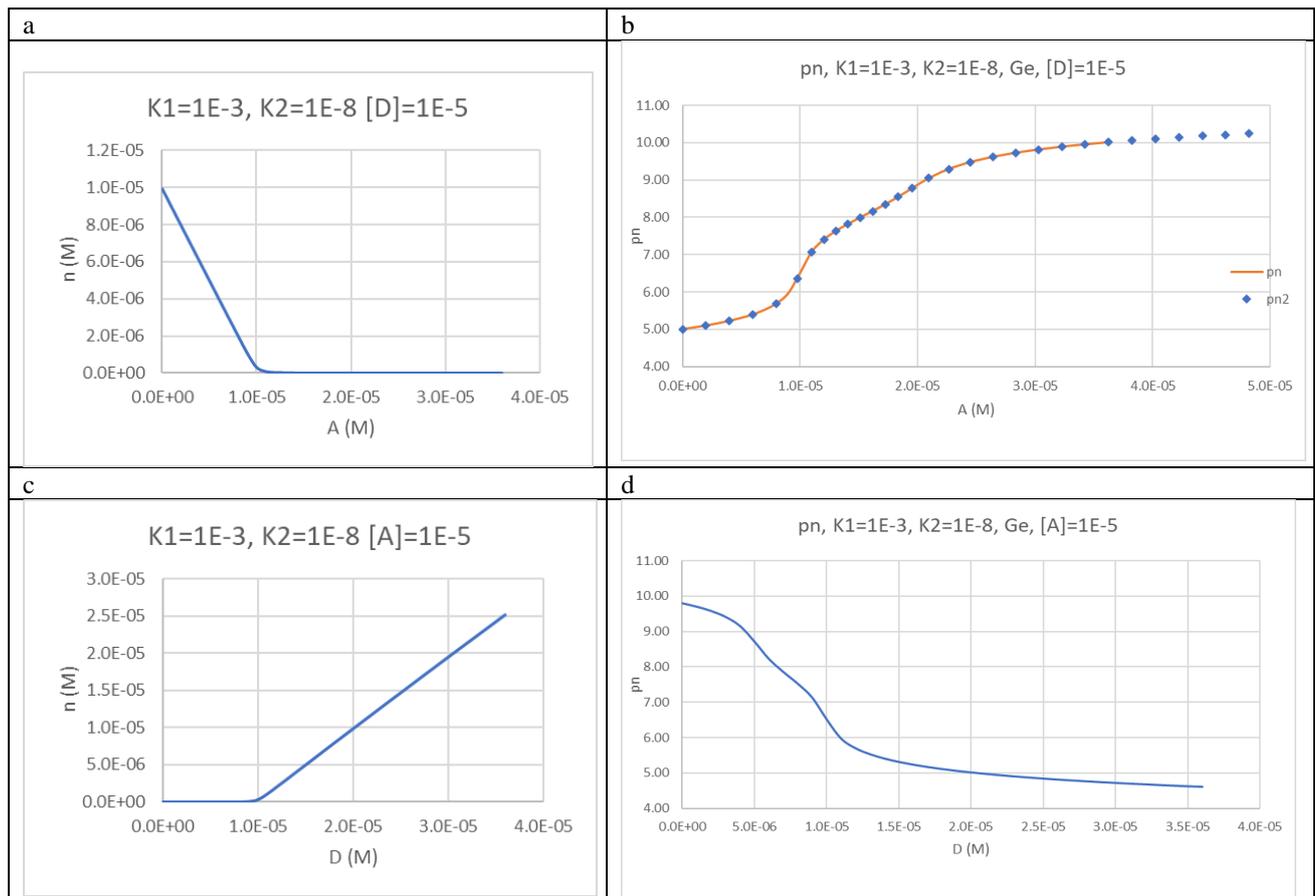


Figure 3 a, b, c, d: Dependence of the electron concentration (n) and (pn) on the change in acceptor and donor concentration. Donor ionization occurs in two stages with the constants K1 and K2. The values of the constants are chosen arbitrarily for better clarity of the curve behavior.

The Case When the General Equation of State Contains Three Ionization Constants

As is known, there is no general solution to the fifth-degree equation in radicals. To represent the dependence of pn on A , we transform the General Equation of State into the dependence of A on n (formula &&&) and plot it (Figure 4).

$$A = [\text{Ge} \cdot K_1 \cdot K_2 \cdot K_3 - n^5 - n^4 \cdot (K_1 + K_2 + K_3) - n^3 \cdot (K_1 \cdot K_2 + K_1 \cdot K_3 + K_2 \cdot K_3 - \text{Ge} - D \cdot K_1) - n^2 \cdot (K_1 \cdot K_2 \cdot K_3 - \text{Ge} \cdot (K_1 + K_2 + K_3) - D \cdot (2 \cdot K_1 \cdot K_2 + K_1 \cdot K_3)) + n \cdot (\text{Ge} \cdot (K_1 \cdot K_2 + K_1 \cdot K_3 + K_2 \cdot K_3) + 3 \cdot D \cdot K_1 \cdot K_2 \cdot K_3)] / (n^4 + n^3 \cdot (K_1 + K_2 + K_3) + n^2 \cdot (K_1 \cdot K_2 + K_1 \cdot K_3 + K_2 \cdot K_3) + n \cdot K_1 \cdot K_2 \cdot K_3).$$

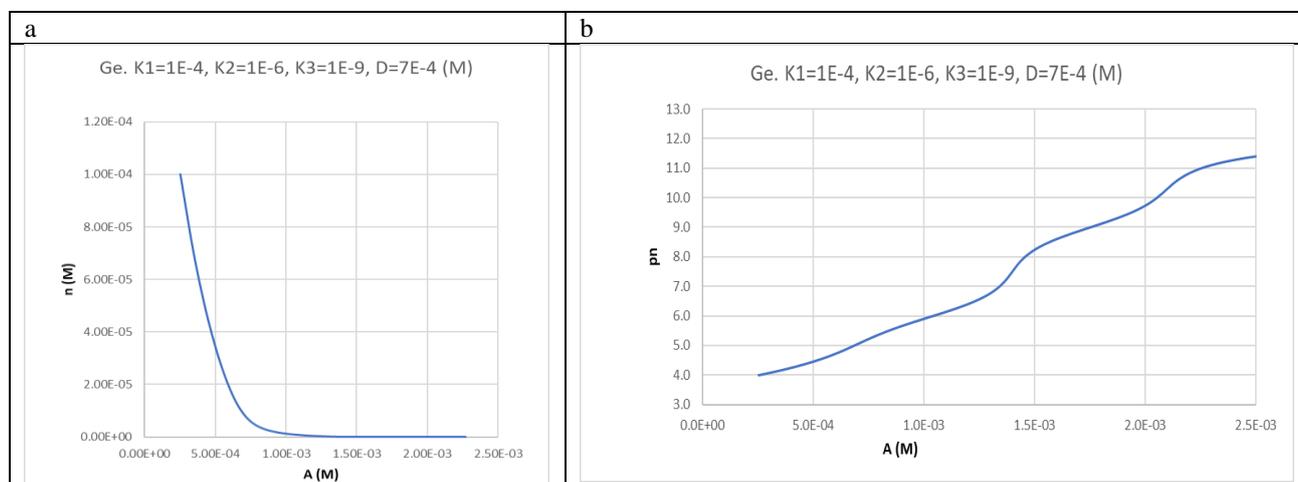


Figure 4 a, b: Germanium. Dependence of the electron concentration (n) and (pn) on the change in acceptor concentration. The General Equation of State contains three ionization constants K_1 , K_2 , and K_3 . The values of the constants are chosen arbitrarily for better clarity of the curve behavior.

The graphs of the $pn=f(A)$ dependence have inflections. At the inflection points, the number of free electrons is equal to the number of holes, these are equivalence points. The number of equivalence points coincides with the number of ionization constants, each ionization stage has its equivalence point. In Figure 1b, the inflection point is visible, the abscissa of the point is equal to 0.001 M of the acceptor impurity, while the starting amount of the donor impurity was also 0.001 M. In Figures 3b and 4b, it is difficult to visually determine the equivalence points with high accuracy, but if we have the General Equation of State, then these points are determined by the algorithm described in the work "Finding Singular Points of the Titration Curve..." (Yefimov, S. 2023).

Appendix# 1

To find the roots of a cubic equation, it is necessary to take several steps and make several changes to variables (Утешев А. 2022).

$$n^3 + a \cdot n^2 + b \cdot n + c = 0$$

let $n = y + k$, and $k = -a/3$ (first changing of variable) \rightarrow
 $y^3 + p \cdot y + q = 0$ were

$$p = b - a^2/3, \text{ and}$$

$$q = 2 \cdot a^3/27 - a \cdot b/3 + c$$

$$y = u + v \text{ and let } u \cdot v = -p/3 \text{ (second changing of variable)}$$

\rightarrow

$$u^3 + v^3 + q = 0$$

$$u^3 \cdot v^3 = -p^3/27 \rightarrow$$

u^3 and v^3 are the roots (t_1, t_2) of the quadratic equation:

$$t^2 + t \cdot q - p^3/27 = 0, \text{ its discriminant is } D.$$

$D = q^2/4 + p^3/27$ – Discriminant of a cubic polynomial. In all cases considered by us, the discriminant of the cubic equation was negative. So, to find the roots, we need to use a complex number: $a + i \cdot b = r \cdot (\cos(\varphi) + i \cdot \sin(\varphi))$ where "i" is the imaginary unit.

Theorem. In the case of $D < 0$, the real roots of the polynomial $y^3 + p \cdot y + q$ are given by the formulas:

$$y_1 = 2 \cdot \sqrt[3]{-p/3} \cdot \cos(\varphi/3)$$

$$y_2 = 2 \cdot \sqrt[3]{-p/3} \cdot \cos(\varphi/3 + 2 \cdot \pi/3)$$

$$y_3 = 2 \cdot \sqrt[3]{-p/3} \cdot \cos(\varphi/3 + 4 \cdot \pi/3) \text{ were } \pi = 3.14 \dots$$

$$\varphi = \arccos(3 \cdot q \cdot \sqrt[3]{-3/p} / (2 \cdot p))$$

The desired n is related to y by the relation: $n = y - a/3$

$n^3 + a*n^2 + b*n + c = 0$		a=	A + K1																
$n = y - a/3$		b=	A*K1 - S - D*K1																
$y^3 + p*y + q = 0$		c=	-S*K1																
$p = b - a^2/3$		$p = A*K - S - D*K - (A+K)*(A+K)/3 = ((A*K^3 - S^3 - D*K^3 - (A+K)*(A+K))/3)$																	
$q = 2*a^3/27 - a*b/3 + c$																			
$d = q^2/4 + p^3/27$																			
$y1 = 2*sqrt(-p/3)*cos(phi/3)$																			
$phi = arccos(3*q*sqrt(-3/p)/(2*p))$																			
$A = (S*K1 + n*(S + D*K1) - n^2*K1 - n^3)/(n^2 + K1*n)$																			
S	6.25E-22	silicon																	
K1	1.75E-05																		
D	1.70E-05	donor																	
#	A	P	q	d	2*(ro)/3	cos(phi)	phi	Y1	Y2	Y3	a/3	n1	n2	n3	pn				
1	0.0E+00	-4.0E-10	2.1E-15	-1.2E-30	2.3E-05	-0.7	2.3	1.6E-05	#####	#####	5.8E-06	1.1E-05	#####	#####	5.0				
2	8.5E-07	-3.9E-10	2.2E-15	-1.1E-30	2.3E-05	-0.7	2.4	1.6E-05	#####	#####	6.1E-06	1.0E-05	#####	#####	5.0				
3	1.7E-06	-3.9E-10	2.2E-15	-9.6E-31	2.3E-05	-0.8	2.4	1.6E-05	#####	#####	6.4E-06	9.4E-06	#####	#####	5.0				
4	2.6E-06	-3.9E-10	2.3E-15	-8.4E-31	2.3E-05	-0.8	2.5	1.5E-05	#####	#####	6.7E-06	8.8E-06	#####	#####	5.1				
5	3.4E-06	-3.8E-10	2.3E-15	-7.3E-31	2.3E-05	-0.8	2.5	1.5E-05	#####	#####	7.0E-06	8.2E-06	#####	#####	5.1				
6	4.3E-06	-3.8E-10	2.4E-15	-6.3E-31	2.3E-05	-0.8	2.6	1.5E-05	#####	#####	7.3E-06	7.6E-06	#####	#####	5.1				
7	5.1E-06	-3.8E-10	2.4E-15	-5.4E-31	2.2E-05	-0.9	2.6	1.5E-05	#####	#####	7.5E-06	7.0E-06	#####	#####	5.2				
8	6.0E-06	-3.8E-10	2.5E-15	-4.6E-31	2.2E-05	-0.9	2.6	1.4E-05	#####	#####	7.8E-06	6.5E-06	#####	#####	5.2				
9	6.8E-06	-3.8E-10	2.5E-15	-3.8E-31	2.2E-05	-0.9	2.7	1.4E-05	#####	#####	8.1E-06	5.9E-06	#####	#####	5.2				
10	7.7E-06	-3.7E-10	2.6E-15	-3.2E-31	2.2E-05	-0.9	2.7	1.4E-05	#####	#####	8.4E-06	5.4E-06	#####	#####	5.3				
11	8.5E-06	-3.7E-10	2.6E-15	-2.6E-31	2.2E-05	-0.9	2.8	1.3E-05	#####	#####	8.7E-06	4.8E-06	#####	#####	5.3				

Figure 1: An example of an EXCEL spreadsheet for calculating the roots of a cubic equation.

As you requested, we develop and supply spreadsheet templates for calculations and plotting curves.

Appendix# 2

To find the roots of a quartic equation $n^4 + a*n^3 + b*n^2 + c*n + d = 0$, it is necessary to take several steps and make several changes to variables (Утешев А. 2022).

Having made the change of variable $n = x - a/4$, we get the equation:

$x^4 + x^2*p + x*q + r = 0$ (#), where

$p = b - 3*a^2/8$

$q = a^3/8 - b*a/2 + c$

$r = d - c*a/4 + b*a^2/16 - 3*a^4/256$

Add and subtract the expression $(x^2*t + t^2/4)$ to (#) to get the sum of two perfect squares:

$(x^2 + t/2)^2 = (t-p)*x^2 - q*x + (t^2/4 - r)$ (##)

The right part of the equation will be perfect square $(t-p)*x^2 - q*x + (t^2/4 - r) \equiv (K*t + L)^2$ at $K = \sqrt{t-p}$, and $L = -q/(2*K)$ if

$D = q^2 - 4*(t-p)*(t^2/4 - r) = 0 = t^3 - p*t^2 - 4*r*t + (4*p*r - q^2)$

$t^3 - p*t^2 - 4*r*t + (4*p*r - q^2) = 0$ This cubic equation is the Ferrari Resolvent.

$t^3 + \alpha*t^2 + \beta*t + \varepsilon = 0$

$\alpha = -p$

$\beta = -4*r$

$\varepsilon = 4*p*r - q^2$

Let's find the root of the Resolvent (see appendix#1), for this, we will make the change of variable $t = y + Y = y - \alpha/3$ and get the equation:

$y^3 + \Pi*y + Q = 0$ (###), where

$\Pi = \beta - \alpha^2/3$

$Q = 2*\alpha^3/27 + \varepsilon - \alpha*\beta/3$

$D = Q^2/4 + \Pi^3/27$ - Discriminant of cubic polynomial

$D < 0 \Rightarrow y = 2*(-\Pi/3)^{1/2}*cos(phi/3)$

Where $\phi = arccos(3*Q*(-3/\Pi)^{1/2}/(2*\Pi))$

if $D > 0$, the only real root is computed using Cardano's formula (Утешев А. 2022). But in all our cases, D was negative.

Now we have one chosen root "y".

Go back to equation (##):

$t = y - \alpha/3$

$K = (t-p)^{1/2}$

$L = -q/(2*K)$

$(x^2 + t/2)^2 = (t-p)*x^2 - q*x + (t^2/4 - r) = (t-p)*x^2 - q*x + (t^2/4 - r) = (K*x + L)^2 \rightarrow$

$(x^2 + t/2)^2 = ((t-p)^{1/2}*x - q/(2*K))^2 \rightarrow$

$x^2 + t/2 = \pm(K*x + L) = \pm((t-p)^{1/2}*x - q/(2*K))$

Now we have two quadratic equations and two discriminants D1 and D2:

$D1 = K^2/4 - (t/2 + L)$, $D2 = K^2/4 - (t/2 - L)$, and hence four roots: $x1, x2, x3$ and $x4$.

We choose one root so that $n = x - a/4 > 0$. Finally, we get the functional dependence $n = f(A, D, K1, K2)$, and the theoretical curve $pn = f(A, D, K1, K2)$.

