THEORETICAL AND COMPARATIVE STUDY OF THE DEPENDENCE OF ELECTRICAL CONDUCTIVITY MECHANISMS IN PURE AND DOPED SILICON ON TEMPERATURE AND IMPURITY CONCENTRATION

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Abstract

This article presents a theoretical and comparative investigation of the physical mechanisms of electrical conductivity in pure and doped silicon as a function of temperature and impurity concentration. Simplified physical models were used to evaluate the intrinsic charge-carrier concentration, electron and hole mobility, and electrical conductivity. The calculations were performed using a silicon band-gap energy of Eg = 1.12 eV, a Boltzmann constant of $k = 8.617\times10^{-5}$ eV/K, and a temperature range of 200–800 K. For pure silicon, the exponential dependence of the intrinsic carrier concentration on temperature was numerically evaluated. For doped silicon, the increase in conductivity with increasing carrier concentration over the range $Nd = 10^{14}$–10^{18} cm^{-3} and the decrease in mobility at high concentrations due to ionized-impurity scattering were comparatively analyzed. The physical significance of the freeze-out, extrinsic, and intrinsic conductivity regimes in doped silicon was substantiated. The results demonstrate the need to consider temperature, doping level, and carrier mobility simultaneously when optimizing electrical conductivity.

Keywords: silicon, semiconductor, electrical conductivity, intrinsic conductivity, doping, donor, acceptor, temperature, charge carriers, mobility, ionized-impurity scattering.

Introduction

Silicon is the principal semiconductor material of modern microelectronics, and its electrical properties depend significantly on temperature, crystal structure, and the concentration of impurity atoms. In pure silicon, free electrons and holes are generated in pairs as a result of the thermal excitation of electrons from the valence band. During doping, donor or acceptor atoms introduce additional energy levels into the crystal and make it possible to control the concentration of majority charge carriers.

According to established theoretical concepts, electrical conductivity is determined not only by the number of carriers but also by their mobility. As temperature increases, the number of intrinsic carriers rises sharply; however, mobility decreases because phonon scattering becomes stronger. In doped crystals, increasing impurity concentration increases the number of carriers, but ionized-impurity centers introduce additional scattering and reduce mobility. Therefore, it is important to evaluate these factors within a unified comparative model.

The aim of the study is to analyze the mechanisms of electrical conductivity in pure and doped silicon based on theoretical models and to evaluate the effects of temperature and impurity concentration numerically and comparatively.

The scientific novelty of the study lies in considering, within a unified comparative approach, the opposing effects of carrier concentration and mobility on electrical conductivity in pure and doped silicon. The dominant conductivity mechanisms under changes in temperature and doping level are identified.

The practical significance of the study is determined by the possibility of theoretically estimating the optimal doping level when selecting the required resistance, conductivity, and operating temperature regime in silicon-based electronic devices.

1. Research Methodology and Calculation Parameters

The study was based on theoretical and numerical modeling methods. For pure silicon under equilibrium conditions, the electron and hole concentrations were assumed to be equal:

$n = p = ni$

The temperature dependence of the intrinsic carrier concentration was calculated using a simplified model:

$Ni(T) = 5.2\times10^{15} \times (T/300)^3/^2 \times \exp[-Eg/(2kT)]$

The calculations used Eg = 1.12 eV and k = 8.617×10^{-5} eV/K. The temperature range was selected as 200–800 K. The purpose of this model is to numerically demonstrate the principal exponential behavior of the intrinsic carrier concentration.

Electrical conductivity was evaluated using the following general equation:

$\sigma = q(n\mu n + p\mu p)$

where q is the elementary charge, n and p are the electron and hole concentrations, respectively, and μn and μp are the electron and hole mobilities.

For doped silicon in the extrinsic regime, under conditions of low compensation and sufficiently ionized impurities, the approximations n≈Nd for n-type material and p≈Na for p-type material were used. The physical relationship that ionized-impurity scattering becomes stronger at high doping levels was taken into account when evaluating the effect of concentration on mobility.

The limitations of the model are as follows: the calculations were performed using simplified parameters; at very high doping levels, degeneracy, band-gap narrowing, and other many-particle effects were not fully taken into account. Therefore, the results describe the principal physical trends.

2. Intrinsic Electrical Conductivity of Pure Silicon

In pure silicon under equilibrium conditions, the electron concentration n and hole concentration p are equal: (n=p=ni). The simplified temperature-dependent expression for the intrinsic carrier concentration has the form

$Ni = \sqrt{(NC\cdot NV)} \times e\hat{}(-Eg / (2k\cdot T))$

where Eg is the band-gap energy, k is the Boltzmann constant, and T is the absolute temperature. As temperature increases, the number of electrons transitioning from the valence band to the conduction band increases, and ni rises sharply [2].

The total electrical conductivity of a semiconductor is the sum of the contributions from electrons and holes:

$\sigma = q(n\mu_n + p\mu_p)$

In pure silicon, the main source of electrical conductivity is the thermal generation of electron–hole pairs. As temperature increases, the probability of electrons in the valence band transitioning to the conduction band increases, and ni rises exponentially. For pure material:

For pure silicon, since n=p=ni:

$\sigma i = qni(\mu_n + \mu_p)$

Table 1. Calculated temperature dependence of the intrinsic carrier concentration in pure silicon

T, K	ni, cm^{-3}
200	2.190e+01
300	2.034e+06
400	7.042e+08
500	2.536e+10
600	2.909e+11
700	1.722e+12
800	6.716e+12

The results in the table show that, within the model, ni increases by several orders of magnitude as the temperature rises from 200 K to 800 K. This is the main physical reason for the sharp increase in the conductivity of pure silicon at high temperatures.

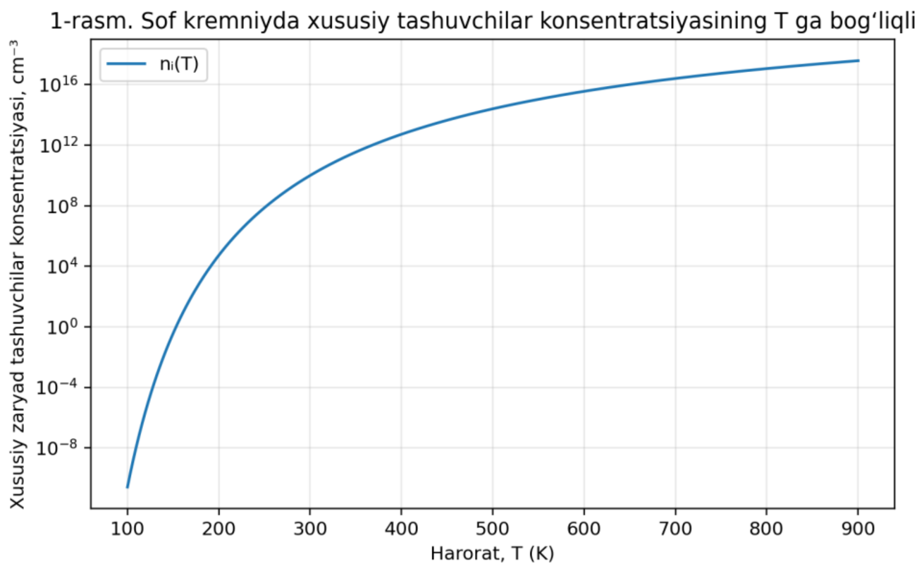

Figure 1. Theoretical temperature dependence of the intrinsic charge-carrier concentration in pure silicon.

3. Electrical Conductivity of Doped Silicon

Doping is the process of introducing controlled amounts of impurity atoms into a crystal lattice. Donor impurities create donor energy levels located close to the conduction band. Much less energy is required to release an electron from this level into the conduction band than is required for excitation across the full band gap. Acceptor impurities, in turn, create acceptor levels close to the valence band and increase the hole concentration.

In the extrinsic regime, under conditions of sufficient donor ionization, for n-type silicon:

$n \approx Nd - Na$

When compensation is neglected:

$n \approx Nd$

4. Temperature-Dependent Conductivity Regimes

In doped silicon, the temperature behavior of carrier concentration and electrical conductivity can be divided into three main regimes:

1) Freeze-out regime. At low temperatures, the ionization degree of donors or acceptors is small. A significant fraction of charge carriers remains bound to impurity centers, and electrical conductivity is low.

2) Extrinsic regime. As temperature increases, most impurities become ionized. In this regime, the concentration of majority carriers is approximately determined by the doping concentration. The subsequent effect of temperature is manifested mainly through mobility via phonon scattering.

3) Intrinsic regime. At sufficiently high temperatures, the concentration of electron–hole pairs generated thermally approaches or exceeds the concentration of carriers produced by impurities. The properties of the material gradually approach those of intrinsic silicon.

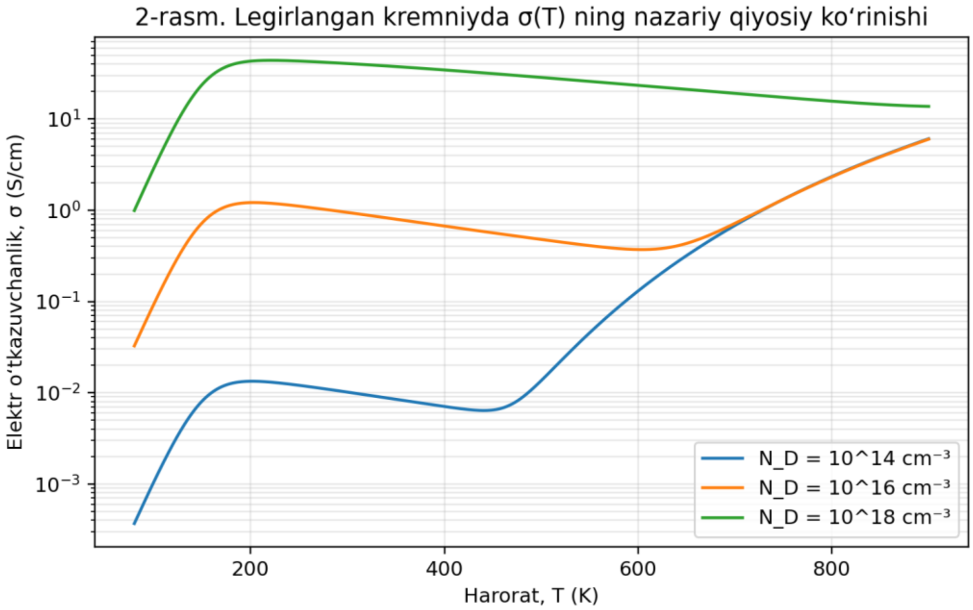

Figure 2. σ(T) dependence of doped silicon at different donor concentrations (theoretical model).

5. Interaction Between Impurity Concentration and Mobility

Increasing the donor concentration over the range 10^{14}–10^{18} cm^{-3} sharply increases the number of carriers. At low and moderate concentrations, this is the main factor responsible for the increase in conductivity. However, as concentration increases, ionized-impurity scattering becomes stronger and restricts the free motion of electrons.

Thus, concentration affects electrical conductivity in two ways: on the one hand, n increases and σ increases; on the other hand, μ decreases and the rate of increase of σ is reduced. These two factors must be considered together when selecting the optimal doping level.

At very high concentrations, the simple n≈Nd model may be insufficient. Degeneracy, changes in the band-gap width, and other high-doping effects must additionally be taken into account. In this work, these effects were not modeled in detail numerically, and the results should be interpreted as simplified theoretical estimates.

In the extrinsic regime around 300 K, when donors are almost completely ionized, the first approximation can be written as $\sigma n \approx q\ Nd\ \mu_n$. If μ_n is assumed to be constant, σ is linearly proportional to the donor concentration. However, in real crystals, increasing Nd strengthens ionized-impurity scattering and reduces electron mobility. Therefore, the dependence of σ on Nd deviates from the ideal linear law.

The theoretical graph in Figure 3 represents precisely this situation: at low and moderate concentrations, increasing the number of carriers effectively increases conductivity, whereas at higher concentrations the decrease in mobility reduces the rate of increase. Therefore, it is important to select the optimal doping level according to the required electrical resistance and current-carrying characteristics of the device.

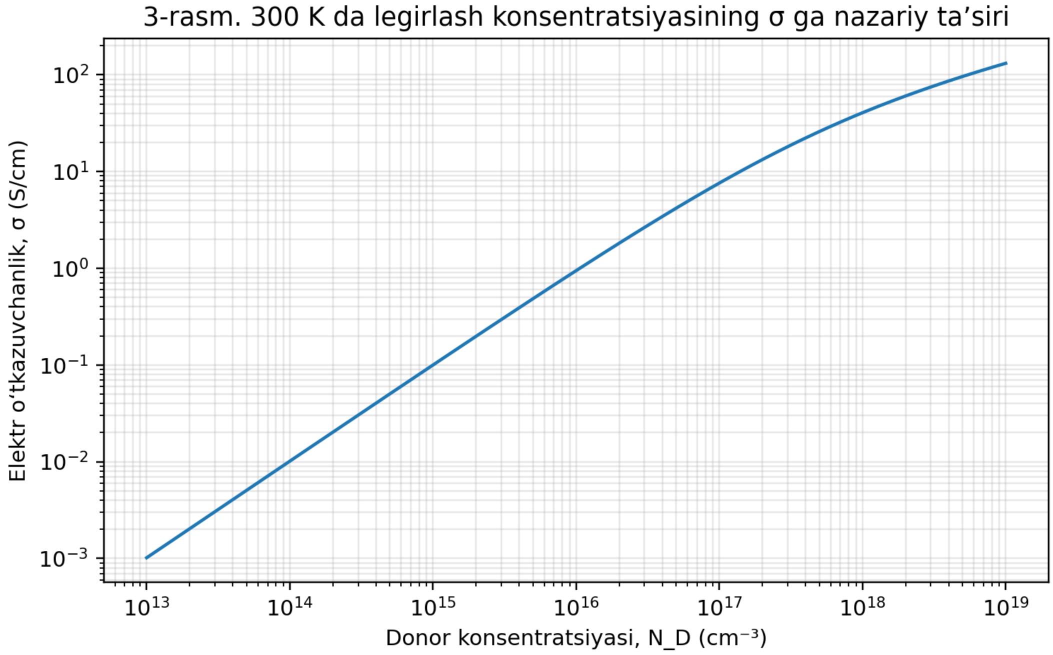

Figure 3. Theoretical variation of electrical conductivity with increasing donor concentration at 300 K.

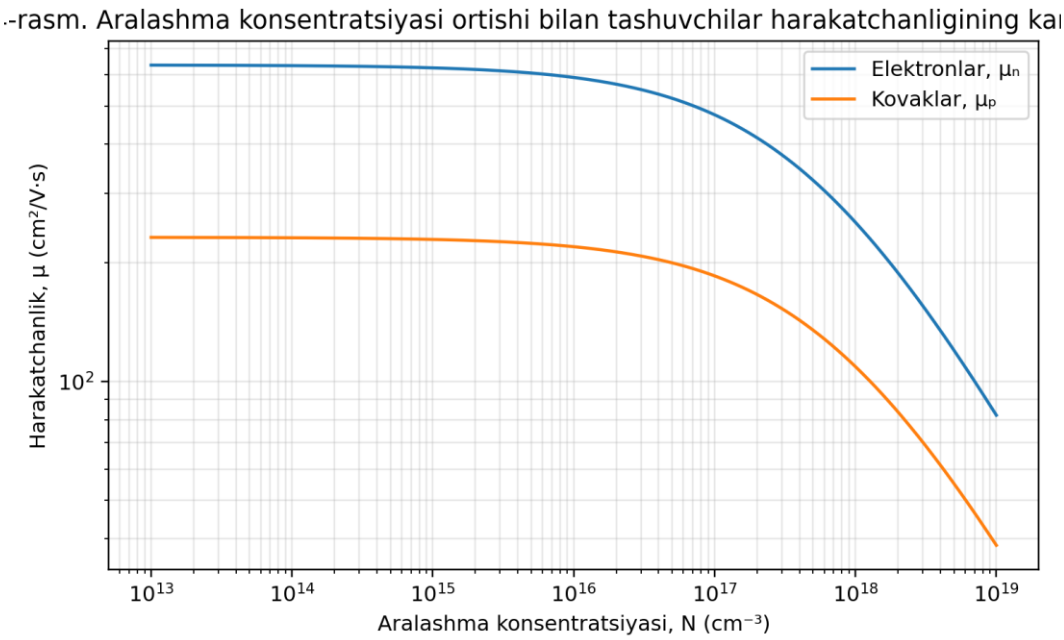

Figure 4. Theoretical decrease in electron and hole mobility with increasing impurity concentration.

6. Comparative Analysis of Pure and Doped Silicon

Property	Pure silicon	Doped silicon
Main carrier source	Thermally generated electron–hole pairs	Donor or acceptor atoms
Main relationship	n=p=ni	n≈Nd or p≈Na (under appropriate conditions)
Temperature effect	ni increases exponentially	Freeze-out, extrinsic, and intrinsic regimes
Effect of concentration	Impurities are nearly absent	Determines the number of majority carriers
Mobility	Mainly affected by phonon scattering	Affected by phonon and ionized-impurity scattering
Applications	High-resistivity and specialized materials	Diodes, transistors, integrated circuits, and sensors

The comparative results show that temperature is the main controlling factor for conductivity in pure silicon, whereas impurity concentration and its degree of ionization are decisive in doped silicon. However, temperature also remains important in doped material: at low temperatures it determines the degree of ionization, at intermediate temperatures it affects mobility, and at high temperatures it determines the generation of intrinsic carriers.

7. Results and Discussion

The calculations showed that the intrinsic carrier concentration in pure silicon depends very strongly on temperature. In the adopted model, ni≈2.19×10^{1} cm^{-3} at 200 K, ni≈2.03×10^{6} cm^{-3} at 300 K, and ni≈6.72×10^{12} cm^{-3} at 800 K. These values are theoretical calculation results within the simplified formula used and demonstrate the principal exponential trend.

In doped silicon, concentrations in the range 10^{14}–10^{18} cm^{-3} lead to a significant increase in conductivity compared with pure silicon. However, as concentration increases, the efficiency of conductivity enhancement decreases because mobility falls. Therefore, the maximum concentration does not always provide the optimal electrical parameters.

The comparative analysis showed that temperature is the dominant factor in pure silicon, whereas in doped silicon, temperature and impurity concentration act in an interconnected manner. At low temperatures, the degree of ionization; at intermediate temperatures, mobility; and at high temperatures, intrinsic generation play the main roles.

The results are based on theoretical modeling. Direct comparison with experimental data, as well as the use of temperature-dependent Eg(T), Nc(T), Nv(T), complete ionization statistics, and accurate μ(N,T) models, could further improve the accuracy of future studies.

Conclusion

1. The main mechanism of electrical conductivity in pure silicon is the thermal generation of electron–hole pairs, and the intrinsic carrier concentration increases exponentially with increasing temperature.

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2. Simplified numerical calculations performed over the range 200–800 K showed an increase in ni by several orders of magnitude; this is a theoretical result confirming the temperature-sensitive electrical properties of pure silicon.

3. In doped silicon, donor and acceptor centers provide the main source of charge carriers. Under the appropriate extrinsic conditions, the approximations n≈Nd or p≈Na can be applied.

4. The temperature-dependent conductivity of doped silicon is characterized by the freeze-out, extrinsic, and intrinsic regimes; the dominant physical mechanisms differ among these regimes.

5. Increasing impurity concentration increases the number of carriers, but mobility decreases due to ionized-impurity scattering. Therefore, the dependence of electrical conductivity on concentration cannot be fully described by a linear model alone.

6. Optimization of electrical parameters requires simultaneous consideration of operating temperature, doping level, carrier type, and the concentration dependence of mobility.

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