

## Dependence of Static Dielectric Constant of Silicon on Resistivity at Room Temperature

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**Abstract:** The static dielectric constant of the heavily doped silicon at room temperature is considered. By using phosphorus as an example, the existing expression for the static dielectric constant at low temperatures is recast into a form suitable for the application at room temperature. This is done by taking into account the contribution of non-ionized impurities at room temperature to the static dielectric constant behavior.

**Keywords:** Static dielectric constant, Heavily doped silicon, Room temperature.

### 1 Introduction

Heavily doped regions are present in every semiconductor device of practical interest today. It is also generally accepted that the existence of heavy doping effects in silicon strongly affects the behavior of all bipolar devices. In most of theoretical works so far, the static dielectric constant in silicon has been assumed to be independent of the impurity concentration at room temperature (although this dependence has been clearly shown to exist at low temperatures). In this paper it is shown that the static dielectric constant of heavily doped silicon at room temperature is not constant.

The idea that static dielectric constant in silicon depends on impurity concentration (the increase of the static dielectric constant with increasing impurity) is not new. This phenomenon has been treated by several authors [1 - 5], all of them having discussed it at low temperatures (except in [6]), where a large number of non-ionized impurity atoms, responsible for the increase in the value of static dielectric constant, are present [7 - 11]. However, in spite of the fact that non-ionized impurities also exist at room temperature [12] the influence of the impurity concentration (resistivity) dependent static dielectric constant (denoted henceforth as ICDSDC) on effects of heavy doping in silicon has been typically neglected.

ICDSDC effect has been clearly pointed out by Castellán and Setz [1]. Considering the contribution of the impurity atoms to the polarization they obtained the static dielectric constant of the impure material as:

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$$\varepsilon_s(N) = \varepsilon_{const} + \frac{N\alpha}{1 - \frac{N\alpha}{3\varepsilon_{const}}}, \quad (1)$$

where  $\alpha$  is the polarizability of the impurity atom,  $\varepsilon_{const}$  the dielectric constant of Si ( $\varepsilon_{const} = 11.7$ ), and  $N$  the concentration on non-ionized impurity atoms. Expression (1) has been used in several works to explain the properties of heavily doped silicon [9], and also when the material is considered to exhibit a metal-nonmetal transition [7].

Dhar and Marshak [5] have extended (1) by taking into account the polarization of the host atoms and its effect on the polarization of the impurity atoms (and vice versa). They obtained the static dielectric constant of the impure material as:

$$\varepsilon_s(N) = \varepsilon_{const} + \frac{N\alpha(\varepsilon_{const} + 2)(4\varepsilon_{const} - 1)}{9\varepsilon_{const} - N\alpha(\varepsilon_{const} + 2)}, \quad (2)$$

where  $\alpha$  is impurity dependent and given by:

$$\alpha = 4\pi \frac{A}{1 - BN^{1/3}}, \quad (3)$$

with  $A$  and  $B$  being constants which, for silicon, depend on the type of impurity. Expression (2) has been shown to be in agreement with experimental data obtained by Castner et al. [7]. It is important to note that (1) and (2) are derived for low temperatures ( $T \rightarrow 0$  K) where all impurity atoms assumed to be non-ionized. This is also in consistency with the experimental conditions of Bethin et al. [2].

The only relationship for ICDSDC which is supposed to be valid at room temperature, up to this author's knowledge, has been given by Andrews et al. [10] as  $\varepsilon_s(N_D) = 11.7$  for the concentration of donors  $N_D < 10^{16} \text{ cm}^{-3}$  and

$$\varepsilon_s(N_D) = C \exp(DN_D), \text{ for } N_D \geq 10^{16} \text{ cm}^{-3}, \quad (4)$$

where  $C$  and  $D$  are constants. Expression (4) has been used in calculations of the electrostatic potential and charge density in graded  $n^+$ -p structures [10]. Also, Theng and Li [11] used (4) for theoretical calculations of the depletion layer width and the depletion capacitance in a heavily doped p-n junction diode. However, although (4) is sufficient to show trends in the static dielectric constant behavior its practical validity is limited for dopant densities up to approximately  $5 \cdot 10^{18} \text{ cm}^{-3}$  [11]. Namely, for larger dopant densities, with the proposed constants  $C$  and  $D$  [10], the exponential nature of (4) indicates a possible divergence of the static dielectric constant, which is similar to the singular behavior of (1) and (2) (usually called "polarization catastrophe") [2, 5]. However, no clear evidence has been given that such an effect would occur in heavily doped silicon at room temperature.

In this paper, the importance of taking into account the non-constant static dielectric constant in heavily doped silicon is pointed out. The most important quantities that characterize heavily doped silicon, such as screening length, standard deviations and density

of states of conduction, valence, donor and acceptor bands are calculated taking into account the impurity concentration dependent static dielectric constant. A simple expression that describes dependence of static dielectric constant on resistivity of phosphorus doped silicon at room temperature is proposed.

## 2 ICSDC model

Here we consider phosphorus - doped silicon in the range  $N_D = 10^{17} \text{ cm}^{-3}$  to  $5 \cdot 10^{20} \text{ cm}^{-3}$  at temperature  $T = 300 \text{ K}$ , with position dependent band structure. Thus, we assume that  $N_A = 0$  and, for thermal equilibrium, we can write [13, 14]

$$N_D = \int_{-\infty}^{+\infty} \max(\rho_c(E), \rho_D(E)) f_n(E, E_F) dE, \quad (5)$$

where  $f_n(E, E_F)$  is Fermi-Dirac function for electrons,  $E_F$  the Fermi energy, while  $\rho_c$  and  $\rho_D$  are the densities of states in the conduction and donor bands, respectively.

In non-degenerate semiconductor conduction and valence band density of states functions are parabolic with respect to energy. At high impurity concentrations (donors in this case), density of states functions have “tails” extending into the band gap. Furthermore, as impurity concentrations increases, the impurity level splits into a large number of close levels, eventually merging into an impurity band with the corresponding density of states. Finally, due to the interactions among carriers and impurity ions, conduction and valence band edges shift towards each other. As a result of these effects, the band structure in heavily doped semiconductor is position dependent and the band gap narrows with increasing impurity concentration.

Expressions that describe non-parabolic conduction and valence band density of states are given by [14]:

$$\rho_c(E) = \frac{4\pi(2m_n^*)^{3/2}}{h^3} \sqrt{\sigma_{CV}} \cdot y\left(\frac{E - E_c}{\sigma_{CV}}\right) \quad (6)$$

and

$$\rho_v(E) = \frac{4\pi(2m_p^*)^{3/2}}{h^3} \sqrt{\sigma_{CV}} \cdot y\left(\frac{E_v - E}{\sigma_{CV}}\right), \quad (7)$$

respectively, with  $y(x)$  given as

$$y(x) = \frac{1}{\sqrt{\pi}} \int_{-\infty}^x \sqrt{x-u} \exp(-u^2) du. \quad (8)$$

Standard deviation  $\sigma_{CV}$ , in equations (6) and (7), is given by [14]

$$\sigma_{CV} = \frac{q^2}{\epsilon_s \epsilon_0} \sqrt{\frac{(N_D + N_A) \cdot \lambda}{4\pi}} \exp\left(-\frac{a_s}{2\lambda}\right), \quad (9)$$

where  $\lambda$  is screening length and  $a_s$  silicon lattice constant.

The donor and acceptor band density of states functions,  $\rho_D$  and  $\rho_A$  respectively, are given by [14]:

$$\rho_{D,A}(E) = \frac{2N_{D,A}}{\sqrt{\pi} \cdot \sigma_{DA}} \exp\left(-\frac{(E - E_{D,A})^2}{\sigma_{DA}^2}\right), \quad (10)$$

where

$$\sigma_{DA} = \frac{q^2}{\varepsilon_s \varepsilon_0} \sqrt{\frac{(N_D + N_A) \cdot \lambda}{4\pi}} \cdot 1.0344 \cdot \exp\left(-\frac{1}{\sqrt{11.3206 \cdot \pi \cdot N_D \cdot \lambda^3}}\right). \quad (11)$$

The total conduction and valence band density of states can be found as  $\rho_e(E) = \max(\rho_c(E), \rho_D(E))$  and  $\rho_h(E) = \max(\rho_v(E), \rho_A(E))$ .

Both  $\rho_c(E)$  and  $\rho_D(E)$  are functions of the screening length  $\lambda$ :

$$\lambda = \frac{1}{q} \sqrt{\frac{\varepsilon_s \varepsilon_0}{\left| \frac{\partial n_o}{\partial E_F} \right| + \left| \frac{\partial p_o}{\partial E_F} \right| + \frac{N_D^+}{kT_{ion}}}}, \quad (12)$$

where  $T_{ion} = 9000$  K [15],  $\varepsilon_0$ ,  $n_o$  and  $p_o$  are permittivity of free space, electron and hole concentration in thermal equilibrium, respectively.

Equation (5) is usually solved for the Fermi level  $E_F$  by assuming total ionization of impurities at room temperature (i.e.  $n_o = N_D = N_D^+$ ) and  $\varepsilon_s = \varepsilon_{const} = 11.7$  [13, 15]. In that case the screening length can be considered as a function of the impurity concentration (curve (a) in Fig. 1) [14]. However, it should be pointed out here that both  $\rho_c(E)$  and  $\rho_D(E)$  in (5) are affected by ICSDC due to the incomplete activation of impurity atoms. Hence, for the case when the static dielectric constant is a function of the concentration of non-ionized impurities  $N$ , (5) can be rewritten as

$$N_D = \int_{-\infty}^{+\infty} \max(\rho_c(E, \varepsilon_s(N)), \rho_D(E, \varepsilon_s(N))) f_n(E, E_F) dE. \quad (13)$$

Since, up to our knowledge, there is a lack of experimental data for ICSDC at room temperature we assume that (2) can be used at  $T = 300$  K with appropriate concentration of non-ionized impurities. Using (3) with  $A = 1.907 \cdot 10^{-20} \text{ cm}^3$  and  $B = 4.698 \cdot 10^{-7} \text{ cm}$  [5] we can rearrange (2) with  $\varepsilon_{const} = 11.7$  as

$$\varepsilon_s(N) = 11.7 + \frac{1.5 \cdot 10^{-16} N}{105.3 - 4.9469 \cdot 10^{-5} N^{1/3} - 3.283 \cdot 10^{-18} N}, \quad (14)$$

with  $N$  being in  $\text{cm}^{-3}$ . Note that (14) is a substantial part of (13).

Obviously, there are two dependent variables ( $N$  and  $E_F$ ) in (13) which implies a family of  $\lambda(N_D)$  dependencies. In order to find a physically valid solution, we employ the

following two constraints on  $\lambda(N_D)$ . The first constraint is that in the whole range of impurity concentrations considered the condition

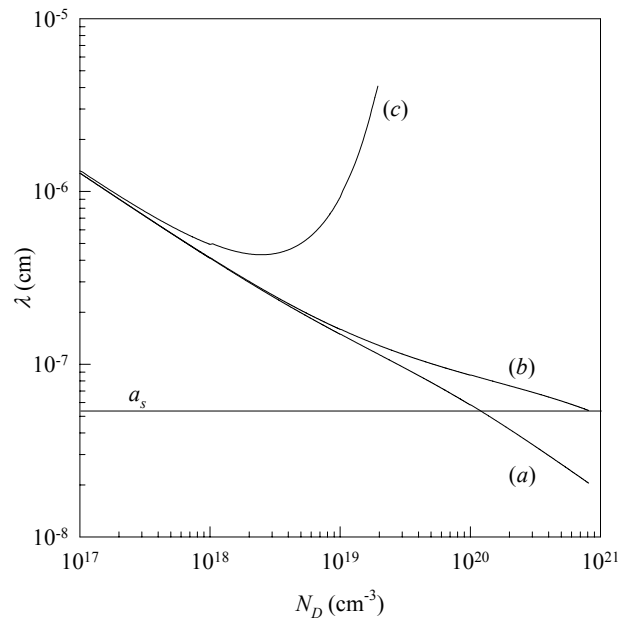
$$\lambda > a_s, \quad (15)$$

is fulfilled. Namely, the static dielectric constant, as a macroscopic quantity, makes sense as long as the screening length stays larger than the lattice constant [16]. It is noteworthy that by using  $\varepsilon_s = \varepsilon_{const} = 11.7$  in (12) for impurity concentrations over  $10^{20} \text{ cm}^{-3}$  the screening length becomes less than the lattice constant, as can be seen from curve (a) in Fig. 1.

The second constraint is that the screening length is assumed to be a monotonically decreasing function, that is

$$\frac{d\lambda}{dN_D} < 0, \quad (16)$$

in order to avoid any possibility of the polarization catastrophe for real impurity concentrations (which is obviously the case when (4) is used, as shown by curve (c) in Fig.1).



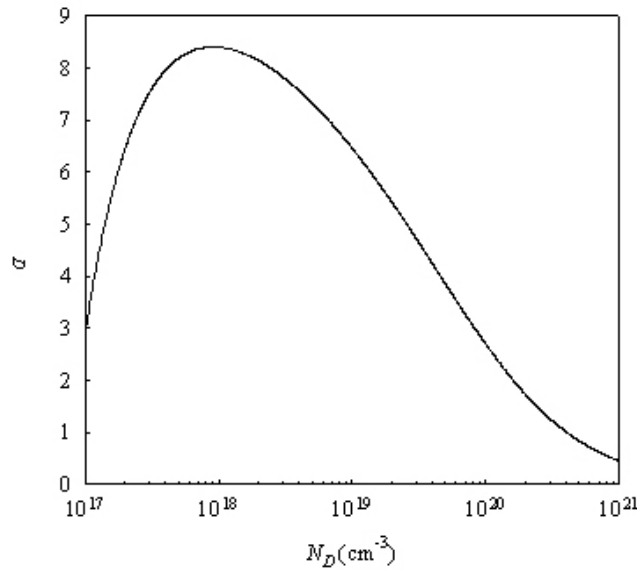
**Fig. 1** - Screening length vs. impurity concentration in silicon at  $T = 300 \text{ K}$ :

(a)  $\varepsilon_s = \varepsilon_{const} = 11.7$ , (b)  $\varepsilon_s = \varepsilon_s(N_D)$  calculated using (14),

(c)  $\varepsilon_s = \varepsilon_s(N_D)$  calculated using (4);  $a_s$  is the silicon lattice constant.

Expression (13), along with (15) and (16), can be numerically solved by a self-consistent procedure as a constrained problem. The solution of (13) which fulfils (15) and

(16) is shown by curve (b) in Fig. 1. It also gives the concentration of non-ionized impurities. Ratio of the concentration of non-ionized impurities to the impurity concentration versus impurity concentration is shown in Fig. 2. It is noteworthy that, although the percentage of non-ionized impurities at higher impurity concentrations is relatively small, their concentration is high enough to affect the static dielectric constant behavior.



**Fig. 2** - Ratio of the concentration of non-ionized impurities to the impurity concentration vs. impurity concentration in silicon at  $T = 300$  K.

By substituting  $N$  shown in Fig. 2 into (14) we obtain the dependence of the static dielectric constant on impurity concentration which is shown in Fig. 3, along with that obtained by using (4). Note that our results also show the general trend of the static dielectric constant to increase but with a much smaller magnitude. Moreover, the occurrence of the polarization catastrophe is avoided for all impurity concentrations of practical interest. For practical calculation purposes the ICDSDC effect for phosphorus can be approximated from curve (b) in Fig. 3 as follows:

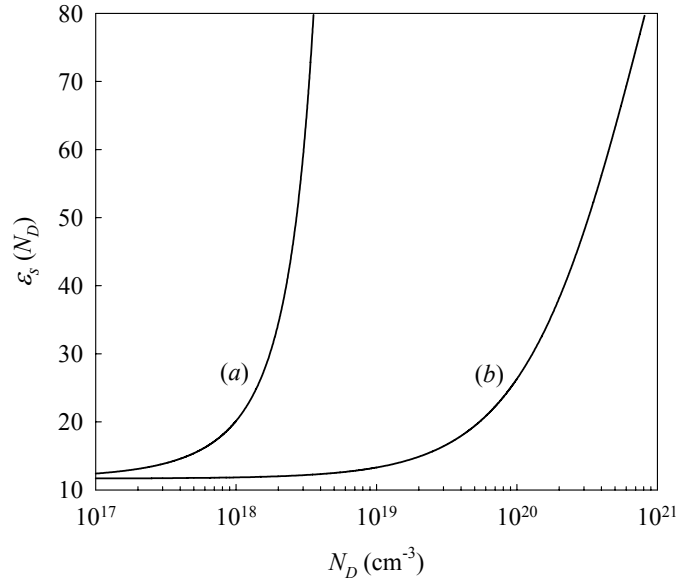
$$\varepsilon_s(N_D) = 11.688 + \frac{1.635 \cdot 10^{-19} N_D}{1 + 1.172 \cdot 10^{-21} N_D}, \quad (17)$$

with  $N_D$  in  $\text{cm}^{-3}$ .

Assuming that the resistivity  $\rho$  ( $\Omega\text{cm}$ ) of phosphorus doped silicon is predominantly affected by electrons as majority carriers, it can be calculated by:

$$\rho \cong \frac{1}{q\mu_n N_D}, \quad (18)$$

where  $\mu_n$  ( $\text{cm}^2/\text{Vs}$ ) is the drift mobility of electrons.



**Fig. 3** - Static dielectric constant vs. impurity concentration in silicon at  $T = 300$  K: (a) calculated from (4); (b) calculated from (7).

In our calculations we have used mobility model which takes into account lattice and ionized impurity scattering, while deviation from ohmic-law field mobility is found to be neglectable. With these assumptions mobility model for electrons  $\mu_n$  ( $\text{cm}^2/\text{Vs}$ ) can be expressed as [17]:

$$\mu_n = 80 + \frac{1350}{1 + \left( \frac{N_D}{1.12 \cdot 10^{17}} \right)^{0.72}}, \quad (19)$$

with  $N_D$  in  $\text{cm}^{-3}$ .

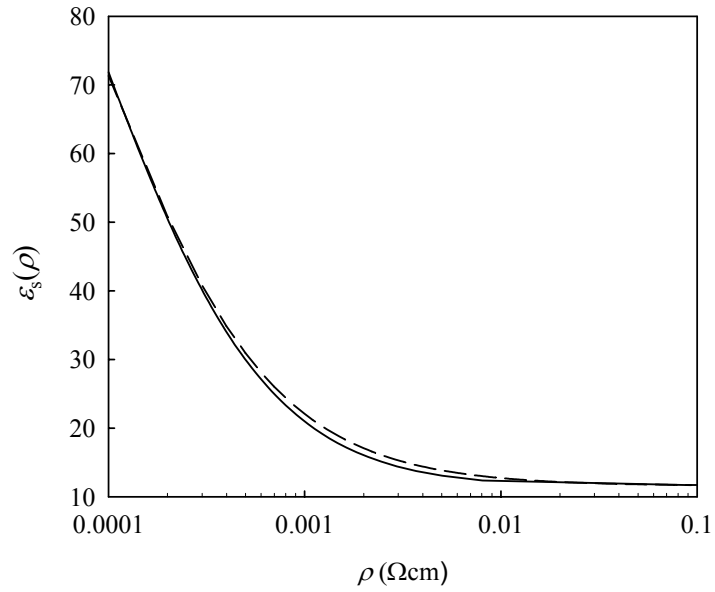
From (17), (18) and (19) we obtain the dependence of the resistivity  $\rho$  in  $\Omega\text{cm}$  on the static dielectric constant (solid line in Fig. 4):

$$\rho = \frac{6.25 \cdot 10^{-3}}{\left( 80 + \frac{1350}{1 + 700 \left( (\varepsilon_s - 11.688) / (163.5 - 1.172 \varepsilon_s) \right)^{0.72}} \right) \frac{\varepsilon_s - 11.688}{163.5 - 1.172 \varepsilon_s}}. \quad (20)$$

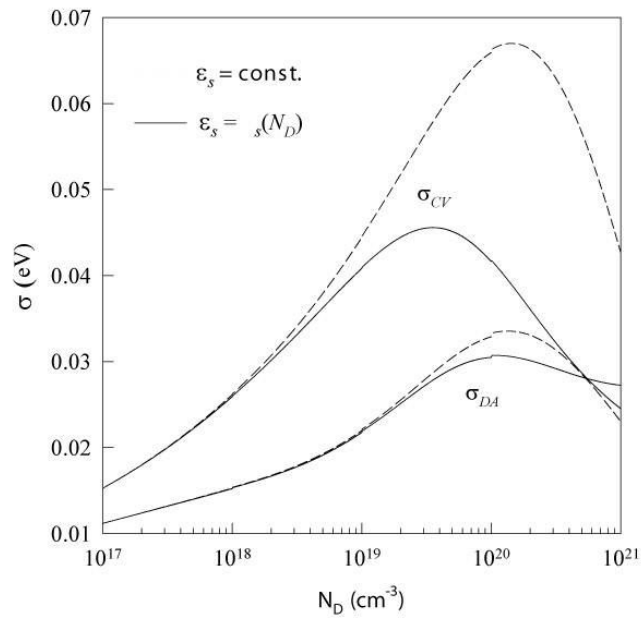
For practical calculation of the dependence of static dielectric constant on the resistivity expression (20) can be approximated as follows (dashed line in Fig. 4):

$$\varepsilon(\rho) = \frac{0.0125 + 11.6\rho}{9.15 \cdot 10^{-5} + \rho}, \quad (21)$$

with  $\rho$  in  $\Omega\text{cm}$ .

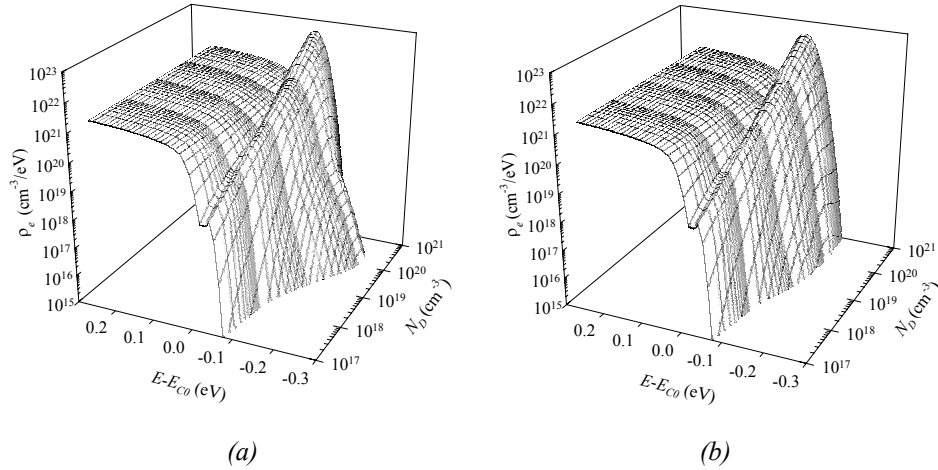


**Fig. 4** - Static dielectric constant of silicon vs. resistivity at  $T = 300$  K: solid line – calculated from (20); dashed line – calculated from (21).

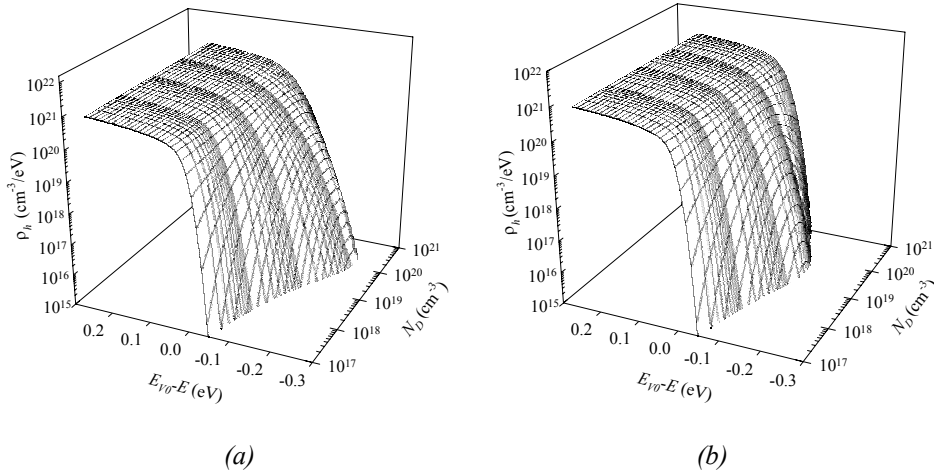


**Fig. 5** - Standard deviations for conduction and valence band and donor and acceptor band vs. impurity concentration in phosphorus doped silicon.





**Fig. 6** - Total conduction band density of states vs. energy in phosphorus doped silicon (a)  $\epsilon_s = \text{const.}$ ; (b)  $\epsilon_s = \epsilon_s(N_D)$ .



**Fig. 7** - Total valence band density of states vs. energy in phosphorus doped silicon (a)  $\epsilon_s = \text{const.}$ ; (b)  $\epsilon_s = \epsilon_s(N_D)$ .

### 3 Impact of ICSDSC on Density of States Functions

Values of static dielectric constant that differ from  $\epsilon_{const} = 11.7$  at high impurity concentrations (Fig. 3.) i.e. at low resistivity of silicon (Fig. 4.) have impact on various semiconductor characteristic variables. For example, calculated standard deviations  $\sigma_{CV}$  - equation (9) and  $\sigma_{DA}$  - equation (11) are shown in Fig.5 for both impurity independent

and impurity dependent static dielectric constant. The difference between these two cases can be easily observed and it implicates the discrepancies between total conduction and valence band density of states functions, which are depicted in Fig.6 and Fig.7, respectively.

#### 4 Conclusion

The well-known effect of the impurity concentration dependent static dielectric constant (ICDSDC) in silicon has been so far analyzed at low temperatures [1, 2, 3, 5] while its existence at room temperature was only a matter of qualitative judgment [6]. A way to obtain a reasonable quantitative estimation for ICDSDC at room temperature is suggested in this paper. Moreover, a framework for the theoretical explanation of density of states in heavily doped silicon is provided.

It is demonstrated that in heavily doped silicon the concentration of non-ionized impurities at room temperature, although small in comparison to the impurity concentration, is high enough to govern the behavior of static dielectric constant. The concentration of non-ionized impurities at room temperature is numerically calculated under constraints related to the screening length. The proposed constraints are established in such a way to retain the macroscopic nature of the static dielectric constant and to avoid the polarization catastrophe in the range of real impurity concentrations. In this procedure, the existing relation for ICDSDC for phosphorus doped silicon at low temperatures [5], is utilized and recalculated taking into account non-ionized impurities at room temperature. As a result, a compact expression for the dependence of static dielectric constant on the resistivity of silicon at room temperature is given.

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