International Journal of Advanced Research and Development
ISSN: 2455-4030; Impact Factor: RJIF 5.24
Received: 25-09-2020; Accepted: 10-10-2020; Published: 26-10-2020
www.advancedjournal.com
Volume 5; Issue 5; 2020; Page No. 34-38

An Evaluation of vector dependence effective screening parameter q_s (Q, T) of Si inversion layer (001) at different temperatures

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Abstract
We have presented the method of evaluation of relative effective screening parameters [$q_s(q,T)/ g(0,0)$] as a function of wave vector q for different temperature for silicon inversion layer Si(001). The evaluation has been done by the theoretical formalism of Egeinluz and Maradudin. The dielectric constant for the physical system in the form of inversion layer has been discussed in a homogeneous medium with dielectric constant k. For small q this dielectric constant leads to the same result. For q>K, the screening effect falls off much more rapidly. This has been taken when the long wavelength dielectric constant at absolute zero is considered for as ideal two-dimensional electron gas of very low density. The present parameter given by eq. (28) is independent of carrier concentration and one with get very unphysical result that at a very low density of carriers continue to screened as effectively as a higher density. The difficulty is removed by eq. (35) because k_r goes to zero as the density goes to zero. This shows that the screening affects a smaller and smaller range of q.

Keywords: Density of state, diffusion energy, Lindhard dielectric function, polarizability, relative screening parameter, Thomas-Fermi approximation

1. Introduction

In this paper we have evaluated the relative screening parameters as a function of q for two dimensional inversion layers of Si (001) at different temperature T. By dynamically two dimensional, we mean that the components of the system are free to move in two spatial dimensions but have their motion constrained in the third dimension. Our principal subject of interest is the systems of electrons in semiconductor inversion and accumulation layers [1, 10]. In the present evaluation, we have taken Si-inversion layer (001) with $N_s=2\times10^{12}$ electrons per cm^2 and the Fermi circle diameter $2K_F = 5.01\times10^6 cm^{-1}$.

2. Mathematical Formula used in the evaluation

a. Density of States

Before going on to a detailed discussion of the two-dimensional electron gas let us recall a basic result for two-dimensional systems, namely the density of states. Because the density of states in n-dimensional wave vector space is $(2\ \pi)^{-n}$, the two-dimensional density of electron states per unit area and unit energy is

$$D\ (E) = 2g_v \frac{1}{(2\pi)^2} 2\pi k \frac{dk}{dE} \qquad (1)$$

Where g_v is a valley degeneracy factor which gives the number of equivalent energy bands and where we have included a factor 2 for spin degeneracy. If the electron excitation spectrum is given by

$$E = E_0 + \frac{\hbar^2 k^2}{2m} \qquad (2)$$

Where *m* is the effective mass, here assumed to be isotropic, we obtain

$$D\ (E) = \frac{g_v m}{\pi\hbar^2},\ E>E_0 = 0,\ E < E_o \qquad (3)$$

Note that the density of states rises abruptly at the energy E_o (in the absence of disorder or level broadening) and is constant for higher energies. There will be additional step increases in the density of states if there are two-dimensional bands at higher energies. When only the lowest band is occupied, the number of electrons per unit area at absolute zero is

$$N_s = \frac{g_v m}{\pi\hbar^2}\ (E_F - E_0) \qquad (4)$$

Where E_F is the Fermi energy. The Fermi surface for the two- dimensional electron system is a curve, also called the Fermi line. In the simplest case of isotropic effective mass it is a circle whose radius is the Fermi wave vector

$$k_F = (2\pi N_s/g_v)^{1/2} \qquad (5)$$

For more complex energy spectra, such as those that obtain for electrons in non-parabolic conduction bands or for holes in warped, non-parabolic valence bands, the density of state must generally be found numerically.

b. Polarizability and screening

The most important property of a two-dimensional electron gas to be considered in this chapter is its response to electromagnetic fields. The simplest example of this kind is the response of the system to a weak, static potential that is slowly varying in space. In addition, we first assume that the electron gas is in a sheet of zero thickness at z = 0 surrounded by homogeneous media with dielectric constants K_{ins} for z < 0 and k_{sc} for z = 0.

The additional electrostatic potential ϕ produced by external source is related to the charge density p by Poisson's equations

$$\nabla . (K\nabla \phi) = —4\pi\rho \qquad (6)$$

where $\rho = \rho_{ext} + \rho$ is the sum of the external charge density and the induced charge density, and k is the dielectric constant, which can be a function of position. In the long-wavelength limit used here, the induced charge density at a point r in the plane z = 0 is a function only of the local potential seen by the electrons, as in the three-dimensional Thomas-Fermi model, and we have

$$\rho_{ind}(r) = -e[N_s(\bar{\phi})-N_s(0)\delta(z)] \qquad (7)$$

Where$\bar{\phi} = \phi(r, 0)$ is the value of the electrostatic potential at r averaged over the electron distribution in z, which is a delta function in the present simplified case. Equation (7) is the two- dimensional analog of the Thomas-Fermi approximation.

A potential $\bar{\phi}$ changes the energy levels by $-e\bar{\phi}$and the separation of the Fermi energy E_F from the bottom of the conduction band by $e\bar{\phi}$. Because we are assuming a weak potential, we can linearize Eq. (7) and find

$$\rho_{ind}(r) = -e \bar{\phi}(r) \frac{dN_s}{d\phi}\delta(z)= -e^2\bar{\phi}(r) \frac{dN_s}{d\phi}\delta(z) \qquad (8)$$

Then Eq. (6) becomes

$$\nabla . (K \nabla \phi) – 2\overline{kq}_s (r) \delta (z) = -4^{\pi}\rho_{ext} \qquad (9)$$

Where ϕ_s is a screening parameter with dimensions of reciprocal length, defined by

$$\bar{\phi}_s =\frac{2\pi e^2}{\bar{K}} \frac{dN_s}{dE_F} \qquad (10)$$

With

$$\bar{K} = \frac{K_{sc} +K_{ins}}{2} \qquad (11)$$

Contrast Eq. (9) with the corresponding equation for linear screening in a homogeneous three-dimensional system:

$$\nabla^2\phi- Q_s^2\phi= - 4\pi\rho_{ext} / k \qquad (12)$$

Where Q_s is the three-dimensional screening parameter, often called q_{TF}. When the external charge is a point charge Ze at the origin, the solution of Eq. (12) is the familiar exponentially screened Coulomb potential $\phi= (Ze/kR) \exp (-Q_sR)$.

To find the screened Coulomb potential for our two-dimensional example, we use a Fourier-Bassel expansion for the potential:

$$\phi (r,z) =\int_0^\infty qA_q(z)J_0(q^r)\, dq \qquad (13)$$

Where J_0 is the Bessel function of order zero and $A_q(z)$ is a function of *q* and *z*, whose value averaged over the delta-function electron distribution is $\bar{A}_q = A_q(0)$

The solution of Eq. (9) when the external charge is a point charge is a point at r = 0, $z = z_o< 0$ is easily obtained. We give here only the value of the Fourier coefficient of the potential in the electron plane as follows:

$$\bar{A}_q = Ze/\bar{k}\, \frac{e^{qz_0}}{q +\bar{q}_s} \qquad (14)$$

For large value of *r*, where $\bar{q}_s (r)>> 0$, the asymptotic form of the average potential seen by the electrons is (Stern, 1967) [11]:

The foregoing example assumed that all the electronic charge was in a plane. Let us now consider the more realistic case of nonzero thickness for the electron layer. The simplest approximation for the charge distribution of electrons is the one first made for inversion layers by Fang and Howard (1966) [12]:

$$G (z) = \frac{b^3}{2}z^2e^{-bz} \qquad (15)$$

This is also the appropriate charge density for electrons in the lowest sub-band for the image potential outside liquid helium (Cole, 1974) if the thickness of the helium-vacuum interface is taken to be zero. Expressions for the parameter *b* and a discussion of the validity of this approximate charge distribution are given. With this charge distribution, the previous considerations are slightly modified: g(z) replaces § (z) in eq. (9), and the average potential felt by the electrons is

$$\bar{\phi}(r) = \int_0^\infty g(z)\, \phi (r, z)\, dz \qquad (16)$$

Whose Fourier-Bessel transform is again called $\bar{A}_q$.

Because of the form of Eq. (16), it is easy to solve Eq. (9) to find the explicit results for the Fourier-Bessel coefficients of the average potential seen by the electrons in the inversion layer (Stern and Howard, 1967) [13]:

$$\bar{A}_q = \frac{Ze}{\bar{K}}\frac{P_0e^{qz_0}}{q+q_sP_{av}+ q_s\delta_kP_0^2},\ z_0 < 0 \qquad (17a)$$

$$\bar{A}_q = \frac{Ze}{\bar{K}_{sc}}\frac{P(z_0)+ \delta_kP_0e^{-qz_0}}{q +q_sP_{av}+ q_s\delta_kP_0^2},\ z_0 > 0 \qquad (17b)$$

Where

$$\delta_k= \frac{K_{sc} - K_{ins}}{K_{sc} + K_{ins}}=\frac{K_{sc}-K_{ins}}{2\bar{K}} \qquad (18)$$

$$q_s= \frac{2\pi e^2}{K_{sc}}\frac{dN_s}{dE_F} \qquad (19)$$

$$P_0 = \frac{b^2}{(b+q)^3} \qquad (20)$$

$$P_{av}= \frac{8b^2+9b^2+3bq^2}{8(b+q)^3} \qquad (21)$$

$$P(z) = \frac{b^3}{(b+q)^3}[e^{-qz} - (a_0 + a_1 z + a_2 z^2)\, e^{-bz}],\ q \neq b$$

$$a_0 = \frac{2q(3b^3 + q^2)}{(b+q)^3},$$

$$a_1 = \frac{4bq(b-q)}{(b+q)^2},$$

$$a_2 = \frac{q(b-q)^2}{b+q}, \qquad (22a)$$

$$P(z) = \frac{1}{8}\ [1 + 2bz + 2b^2 z^2 + \frac{4}{3} b^3 z^3]\, e^{-bz},\ q = b \qquad (22b)$$

Note that in the limit of large *b* the results in Eq. (17a) reduce to those for the extreme two-dimensional limit given in Eq. (13)

Equation (17) can be used to calculate the Born-approximation cross section for scattering of electrons in the lowest sub-band by charged centers in the oxide and in the semiconductor. Recently [10, 16] there have been calculations which treat the scattering centers in a more sophisticated way by taking into account the occupation of the bound state in the presence of a screening charge distribution. The results given above are the two- dimensional analog of the conventional Brooks-Herring treatment of ionized impurity scattering in semiconductors (Smith, 1978) [17].

Let us now look more closely at the screening parameter q_s, defined in Eq. (20), which gives the screening effects in the long wavelength, static approximation, and on the related parameter q_s, defined in Eq. (10), which enters in the extreme two-dimensional limit. We have

$$K_{sc} q_s = \overline{Kq}_s = \frac{2\pi e^2 N_s}{E_d} \qquad (23)$$

$$\text{Where } E_d = \frac{N}{(dN_s/dE_F)} \qquad (24)$$

Is called the diffusion energy because it enters in the generalized Einstein relation (Spenke, 1955) [18]

$$D = \frac{E_d}{e}\mu \qquad (25)$$

Connecting the diffusion coefficient D and the mobility μ.

For the simple two-dimensional density of states given by Eq. (3), we have (Stern and Howard, 1967) [13]

$$\frac{E_d}{K_B T} = [1 + exp\left[\frac{E_0 - E_F}{K_B T}\right]]\ln[1 + exp\left[\frac{E_0 - E_F}{K_B T}\right]] \qquad (26)$$

At low temperature, when $E_F - E_0 >> k_B T$, the diffusion energy $E_d \sim E_F - E_0$ and

$$q_s = g_v/a^*,\ a^* = \frac{k_{sc}\hbar^2}{me^2} \qquad (27a)$$

$$\bar{q}_s = g_v/a^*,\ a^* = \frac{k\hbar^2}{me^2} \qquad (27b)$$

Where a* and a* are the effective Bohr radii using the semiconductor dielectric constant and the average of the semiconductor and insulator dielectric constants, respectively. At high temperatures the diffusion energy is $E_d >> 7_B T$ and

$$Kq_s = \overline{Kq}_s = \frac{2\pi e^2 N_s}{K_B T} \qquad (28)$$

Note, however, that at high temperature more than one sub-band will be populated with carriers and the expressions given here must be generalized. Such generalizations have been given by Stern and Howard (1967) [13] and more fully by Siggia and Kwok (1970) [19], and have been applied to mobility calculations by Stern (1978a) [20] and by Mori and Ando (1979) [21].

The results given so far in this chapter have assumed that the potentials being screened are very slowly varying in space and static in time. In several kinds of problems, including the calculation of bound states and the scattering of carriers at elevated temperatures or in more than one sub-band, this approximation no longer suffices. The simplest approximation that gives the response of the system to shorter wave lengths and to time varying potentials is the self-consistent or random phase approximation, in which each electron is assumed to move in the external field plus the induced field of all electrons. This is the model which leads to the famous Lindhard (1954) [22] dielectric function for a three- dimensional electron gas. It ignores dynamical correlation effects and is known to lead to errors in various quantities such as the pair correlation function (Jonson, 1976) [23], but it is nevertheless widely used because it gives the simplest nontrivial result for the linear response of the system to an external field.

The polarization induced by one component $F(q, \omega) = F_0 \exp(q.r - i\omega t)$ of the total (external plus induced) electric field acting on the sheet of electrons at z = 0 can be written

$$P(q,\omega) = \chi(q, \omega)\, F(q, \omega)\, \delta(z) \qquad (29)$$

Where χ is the polarizability of the layer, given by Ehrenreich and Cohen (1959) [24]:

$$\chi(Q, \omega) = \frac{e^2}{q^2 L^2} \lim_{\alpha \to 0} \sum \frac{f_0(E_k) - f_0(E_{k+q})}{E_{k+q} - E_k - \hbar\omega - i\hbar\alpha} \qquad (30)$$

f_0 Is the Fermi-Dirac occupation probability, L^2 is the normalization area, and the sum is over all one-electron states of wave vector *k* and energy E_k.

For an isotropic two-dimensional electron gas with energy levels $E_k = \hbar^2 k^2/2m$ and Fermi wave vector k_F, Eq. (30) evaluated at absolute zero gives $\chi = \chi_1 + i\chi_2$, where (Stern, 1967) 11

$$\chi_1 = \frac{2me^2 N_s}{\hbar^2 K_F q^3}\left\{\frac{q}{K_F} - C_- \left[\left[\frac{q}{2K_F} - \frac{mk_F\omega q}{\hbar}\right]^2 - 1\right]\right.$$

$$- C_+ \left[\left[\frac{q}{2K_F} + \frac{mk_F\omega q}{\hbar}\right]^2 - 1\right]^{1/2} \qquad (31a)$$

$$\chi_2 = \frac{2me^2 N_s}{\hbar^2 K_F q^3}\{-D_-\left[1 - \left[\frac{q}{2K_F} - \frac{mk_F\omega q}{\hbar}\right]^2 - 1\right]$$

$$-D_{+}\left[1-\left[\frac{q}{2K_F}-\frac{mk_F\omega q}{\hbar}\right]^2-1\right] \qquad (31b)$$

$$C_{\pm}=\left[\frac{q}{2K_F}\pm\frac{mk_F\omega q}{\hbar}\right]$$

$$D_{\pm}=\left[\frac{q}{2K_F}\pm\frac{mk_F\omega q}{\hbar}\right]>1 \qquad (31c)$$

$$C_{\pm}=0, D_{\pm}=1, \left[\frac{q}{2K_F}\pm\frac{mk_F\omega q}{\hbar}\right]<1 \qquad (31d)$$

These results are best understood by looking at a number of special cases. The simplest is the static, long wave length limit considered above. Then we find, for $\omega = 0$, $q \sim 0$, that

$$\rho_{ind} = -q^2 \chi(q)\phi(r)\delta(z)$$

$$= -\frac{N_s e^2}{E_F}\bar{\Phi}(r)\,\delta(z) \qquad (32)$$

In agreement with Eq. (8). More generally, § (z) is replaced by g (z).

The dielectric constant for the physical system we are dealing with will be nonlocal function in general (Dahl and Sham, 1977; Eguiluz and Maradudin, 1978a, 1978b) [25, 27] but can be expressed in a simple form when the inversion layer is a sheet of charge in the plane z = 0 embedded in a homogeneous medium dielectric constant *k*. Then one can define a dielectric constant for longitudinal excitation within the plane of electrons to be (Stern, 1967) [11]

$$K(q,\omega) = K + 2\pi\beta\chi(q,\omega) \qquad (33)$$

Where $p^2 = q^2 - K\,\omega^2/c^2$. For the corresponding results in a more general case (Dahl and Sham, 1977) [25].

For static fields Eqs. (32) And (34) give

$$K(q,\omega) = K\left[1+\frac{q_s}{q}\right], \; q \le 2K_F, \; ½$$

$$= K\left[1+\frac{q_s}{q}\left\{1-\left[\frac{2K_F}{q}\right]\text{^}2\right\}\right], \; q > 2K_F, \qquad (34)$$

For small *q*, this dielectric constant leads to the same results that we obtained in a different way above. For $q > 2K_F$, the screening effects fall off much more rapidly. This removes a conceptual difficulty that arises when the long wave length dielectric constant at absolute zero is considered for an ideal two-dimensional electron gas very low density. The screening parameter, given by Eq. (28), is independent of carrier concentration, and we would have the unphysical result that a very low density of carriers continues to screen as effectively as a higher density. This difficulty is removed by Eq. (36), because k_F goes to zero as the density goes to zero, so that the screening affects a smaller and smaller range of *q*. In a real system, finite temperature and band tailing effects will also limit the screening at low electron densities.

A more important effect of the cutoff of screening for large wave vectors is the change of slope of the dielectric function at $q = 2k_F$. This change leads to Friedel oscillations in the response of the system to a localized disturbance, just as in three dimensions. The leading term in the potential at large distances for a screened Coulomb potential induced by a point charge Ze in the same plane as the sheet of electrons is (Stern, 1967) [11]:

$$\bar{\phi}(r) \sim -\frac{Zeq_{s'}}{k}\frac{4K_F^2}{(2K_F+q)^2}\frac{\sin(2K_F r)}{(2K_F r)^2} \qquad (35)$$

Similar results have been found for three-dimensional semiconductors with cylindrical energy bands by Roth, Zeiger and Kaplan (1966; Gabovitch *et al.*, 1978, for metals) [28, 29] for carrier- induced magnetic interactions in two-dimensional systems by Fischer and Klein (1975) [30] and, apart from a phase difference, for the interaction between absorbed atoms induced by the response of a partially filled band of surface states, by Lau and Kohn (1978) [31].

Maldague (1978a) [32] showed how the temperature dependent static polarizability can be obtained from the values at absolute zero. His results can be written

$$\chi(Q,\omega; T,\mu) = \int_0^\infty \frac{\chi(q,\omega;0,\mu')}{4k_B T\cosh^2\left\{\frac{\mu-\mu}{2K_B T}\right\}}d\mu' \qquad (36)$$

Where Tis the absolute temperature and jli is the chemical potential. The high temperature limit of the static dielectric function was found by Fetter (1974b) [33] to be

$$K(q,0) = \bar{k}\left[1+\frac{q_s(q)}{q}\right],$$

$$q_s(Q) = \frac{2\pi N_s e^2}{K_B T}\, g_1(q\lambda),$$

$$\lambda = \left[\frac{2\pi\hbar^2}{mk_B T}\right]_{½}$$

$$g(\chi) = \frac{2\pi^{1/2}}{\chi}\phi\left[\frac{\chi}{4\pi^{1/2}}\right] \qquad (37)$$

$$\phi(y) = -\pi^{½}\,\wp\int_{-\infty}^{\infty}dz\,\frac{e^{-z^2}}{y-z}$$

where $\wp$ denotes principle value, is the real part of the plasma dispersion function as defined by Fetter and Walecka (1971), whose definition differs by a factor -1 from that of Fried and Conte (1961) [34]. Note that $g_1(0)$ =l, and that Eq. (38) can give misleading results unless the occupations and spatial extents of the higher-lying sub-bands are taken into account. The wave vector dependence of the effective screening parameter in a single sub-band at absolute zero and at higher temperatures as calculated by Stern (1980b) [35].

3. Discussion of the Results

In this chapter, we have presented the method of evaluation of relative effective screening parameters $[q_s(q,T)q_s(0,0)]$ as a function of wave vector *q* for different temperature for silicon inversion layer Si(001). The evaluation has been done by the theoretical formalism of Egeinluz and Maradudin [35]. Here the dielectric constant for the physical system in the form of inversion Layer has been discussed in a homogeneous medium with dielectric constant k. The expression has been given in Eqs. (34) and (35). For small *q* this dielectric constant leads to the same result. For q>2K, the screening effect falls off much more rapidly. This has been taken when the long wavelength dielectric constant at absolute zero is considered for as ideal two-dimensional electron gas of very low density. The present parameter given by eq. (28) is independent of carrier concentration and one with get very unphysical result that at a very low density of carriers continue to screened as effectively as a higher density. The difficulty is removed by equation (35) because k_F goes to zero as the density goes to zero. This shows that the screening affects a smaller and smaller range of *q*. Our calculation for relative screening parameter shows that $[q_s(q,T)/q_s(0,0)]$ decreases as a function of as for large temperature. Its value is maximum at 10K and minimum at 80K. Its decrease becomes much faster of the $q > 2k_F$. Our results are consistent with the other theoretical workers [37, 40].

Table 1: Evaluation of relative screening parameters as a function of wave vector for silicon inversion layer Si (001) for different temperatures $N_S = 2\times10^{12}$ electrons per $cm^{2,}$ $2K_f = 5.01\times 10^6\ cm^{-1}$

Wave Vector $q(10^6cm^{-1})$	Relative screening parameters $[q_s(q/T)/q_s(0,0)]$			
	T=10K	T=20K	T=40K	T=80K
1.0	1.123	1.035	1.003	0.962
1.5	1.104	1.022	0.928	0.805
2.0	1.087	1.006	0.813	0.713
2.5	1.068	0.952	0.632	0.586
3.0	1.059	0.868	0.509	0.498
3.5	1.047	0.693	0.386	0.362
4.0	1.038	0.534	0.296	0.318
4.5	1.026	0.428	0.242	0.252
5.0	1.005	0.329	0.208	0.218
5.5	0.956	0.261	0.192	0.192
6.0	0.723	0.224	0.176	0.178
6.5	0.628	0.203	0.158	0.163
7.0	0.531	0.196	0.142	0.148
8.0	0.438	0.182	0.113	0.126

4. Conclusion

Our calculation for relative screening parameter shows that [gs (q,T)/9s(0,0)] decreases as a function of as for large temperature. Its value is maximum at 10K and minimum for 80K. Its decrease becomes much faster of the $q > 2k_F$.

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