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# Theory of the mobility of electrons in a semiconducting-surface inversion layer

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The dc mobility for the lowest subband electrons in a Si(100) surface inversion layer have been caluculated by the standard memory-function approach and also by the Boltzmann equation. We show that the results obtained from these two methods do not agree with each other when the temperature becomes finite. The scattering mechanisms due to the oxide charges at the semiconductor-insulator interface and the surface roughness are considered. Our numerical results seem to indicate that the dc resistivities derived from both methods can be fitted to agree with experiments at low temperature if the parameters involved are varied slightly.

It is well known that the memory-function approach[1] has been quite successful in its application to calculate the resistivity of an ideal metal whose Fermi surface is spherical. For example, the resistivity formula obtained from the memory-function approach agrees with that from the Boltzmann equation[2] at low temperature if the scattering mechanism of electrons are due to impurities and phonons. However, at higher temperature, especially when the temperature $T$ is comparable to the Fermi energy $E_F$ of the system, the comparison between the results of these two methods has never been made. In this article we shall show that the dc mobility obtained from the memory function approach is not unique and its expression is determined entirely by the method of expansion used here. We shall also show that the dc mobility obtained from the standard high-frequency expansion method used in the work of Götze and Wölfle[1] no longer agrees with the result from the Boltzmann equation[3] whenever the temperature $T$ becomes finite. The transport relaxation rates obtained from these two approaches will be calculated numerically as a function of $T$ for electrons in Si(100) surface inversion layer. The scattering mechanisms due to the oxide charges at the semiconductor-insulator interface and the surface roughness will be considered. Our numerical results seem to indicate that the dc resistivities derived from both methods can be fitted to agree with experimental measurements[4] if the parameters involved are varied slightly.

First let us briefly review the procedure to obtain the dc mobility from the standard memory function approach. As it has been shown that the dynamic conductivity derived from the current-current correlation function can be written as [5]

$$\sigma(\omega)=\frac{i}{\omega}\frac{Ne^2}{m}\left[1+\frac{M(\omega)}{\omega}\right], \tag{1}$$

$$M(\omega)=\frac{1}{Nm\omega}\sum_q q_x^2\,|v(q)|^2[s(q,\omega)-s(q,0)], \tag{2}$$

where $N$ is the electron concentration, $m$ and $e$ are, respectively, the effective mass and the charge of an electron. $|v(q)|^2$ is the scattering matrix which contains both the mechanisms due to charged impurities and surface roughness. Its expression will be given later. $s(q,\omega)$ is the density-density correlation function for conduction electrons. On the other hand, the Drude formula for conductivity has the expression

$$\sigma(\omega)=\frac{iNe^2}{m[\omega+i/\tau(\omega)]}\ . \tag{3}$$

The relaxation time $\tau(\omega)$ can be obtained by comparing Eq. (3) with Eq. (1). If $M(\omega)$ is evaluated to the lowest order in the scattering matrix, we have $1/\tau(\omega)=iM(\omega)$. In the following, what we are interested in is the limit of $\omega\rightarrow 0$. From Eq. (3) the dc conductivity can be written as $\sigma=Ne^2/m\langle 1/\tau\rangle^{-1}$; here $\langle 1/\tau\rangle^{-1}=1/\tau(0)$. If the density-density correlation function $s(q,\omega)$ in Eq. (2) is evaluated in the random-phase approximation[6] (RPA) for electrons in a semiconducting surface inversion layer, $\langle 1/\tau\rangle=iM(0)$ can be shown to have the form

$$\left\langle\frac{1}{\tau}\right\rangle=\int_0^\infty dE\,\frac{1}{\tau(E)}\left[\frac{E}{E_F}\right]\left[-\frac{\partial}{\partial E}n(E)\right], \tag{4}$$

with

$$\frac{1}{\tau(E)}=\frac{E_F m}{N\pi}\int_0^{2\pi}\left|\frac{v(q)}{\epsilon(q,0)}\right|^2(1-\cos\phi)\,d\phi\,, \tag{5}$$

where $n(E)=[\exp(E-\mu)/T+1]^{-1}$ is the Fermi function and $\mu=T\ln[\exp(N\pi/2mT)-1]$ is the chemical potential. $q=2\sqrt{2mE}\,\sin(\phi/2)$ and $\epsilon(q,0)$ is the static dielectric function in RPA (Ref. 6):

$$\epsilon(q,0)=1+v_e(q)\frac{m}{\pi}\int_0^1\frac{d\xi}{\sqrt{1-\xi}}\,\frac{1}{e^{(\eta\xi/4-U)\xi_0}+1}\,, \tag{6}$$

where $\eta=q^2/2mE_F$, $U=\mu/E_F$, $\xi_0=E_F/T$, $v_e(q)$ is the effective electron-electron interaction, $m=0.195m_0$ is the effective mass for electrons in the Si(100) surface, and $m_0$ is the free-electron mass. The mobility $\mu_D$ can therefore be obtained from the conductivity $\sigma$, for example, $\mu_D=\sigma/Ne$ and we have

$$\mu_D=\frac{e}{m}\left\langle\frac{1}{\tau}\right\rangle^{-1}. \tag{7}$$

The expression for $\mu_D$ in the above equation is directly the consequence of the classical Drude conductivity formula defined in Eq. (3). However, according to the Boltzmann Eq. (2) the conductivity at finite $\omega$ can be written as

$$\sigma(\omega)=ie^2\sum_k\frac{(v_k^x)^2}{\omega+i/\tau_k(\omega)}\left[-\frac{\partial n(k)}{\partial E(k)}\right], \tag{8}$$

where $\tau_k$ and $v_k^x$ are, respectively, the relaxation time and the $x$-component velocity of the electron with momentum $\vec{k}$. If $\tau_k(\omega)$ is independent of $\vec{k}$, Eq. (8) reduces back to the Drude formula of conductivity as defined in Eq. (3). The expression for $1/\tau_k(\omega)$ can also be obtained by comparing Eq. (8) with Eq. (1); in the limit of $\omega\to 0$ we have

$$\frac{m}{N}\sum_k\frac{(v_k^x)^2}{\tau_k(0)}\left[\frac{\partial n(k)}{\partial E(k)}\right]=iM(0)\,. \tag{9}$$

Transforming the summation over $\vec{k}$ to an integration over $E(k)=k^2/2m$ in the above equation, it is straightforward to show that $1/\tau_k(0)$ has the exact expression as $1/\tau(E)$ [Eq. (5)] with $E$ defined as $E=E(k)$. The dc conductivity obtained from Eq. (8) can then be written as $\sigma=Ne^2/(m\langle\tau\rangle)$ and $\langle\tau\rangle$,

$$\langle\tau\rangle=\int_0^\infty dE\,\tau(E)\left[\frac{E}{E_F}\right]\left[-\frac{\partial}{\partial E}n(E)\right]. \tag{10}$$

The mobility formula $\mu_B$ obtained by comparing Eq. (1) with Eq. (8) is thus different from that in Eq. (7):

$$\mu_B=\frac{e}{m}\langle\tau\rangle\,. \tag{11}$$

This result has also been obtained by Stern,[3,7] who used a different method. It is easy to see that $\mu_B=\mu_D$ at $T=0$ K. However, we shall show below that the values of $\mu_D$ and $\mu_B$ will be different when $T$ becomes finite.

In the following the mobilities $\mu_D$ and $\mu_B$ will be studied numerically at finite temperature. The scattering of electrons due to oxide charges and surface roughness will be considered here; the scattering amplitude $|v(q)|^2$ that appeared in Eq. (5) can then be written as

$$|v(q)|^2=n_I|v_i(q)|^2+|v_{\rm sr}(q)|^2\,, \tag{12}$$

where $v_i(q)$ and $v_{\rm sr}(q)$ are, respectively, corresponding to the interaction of electrons with charged impurities and surface roughness. $n_I$ is the impurity concentration. The derivation of $v_i(q)$ has been shown in Ref. 6 and its explicit expression will not not be given here. In our following numerical calculation, the surface roughness potential $v_{\rm sr}(q)$ of Matsumoto and Uemura[8] will be used:

$$v_{\rm sr}(q)=\frac{4\pi e^2}{\bar{\epsilon}_s}\left[\frac{n}{2}+n_{\rm dep}\right]\Delta d\exp(-d^2q^2/8)\,. \tag{13}$$

Here $\bar{\epsilon}_s=\frac{1}{2}(\epsilon_s+\epsilon_0)$, $\epsilon_s=11.8$ and $\epsilon_0=3.8$ are the dielectric constants for silicon and oxide. $n_{\rm dep}$ is the effective charge density in the depletion layer. $\Delta$ and $d$ are, respectively, the mean-square height and the lateral correlation length.

The results of our numerical calculation for Si(100) surface inversion layer are shown in Fig. 1 for $n=2.0\times10^{12}\,{\rm cm}^{-2}$ and $n_{\rm dep}=0.3\times10^{12}\,{\rm cm}^{-2}$. There we have assumed that the charged impurity

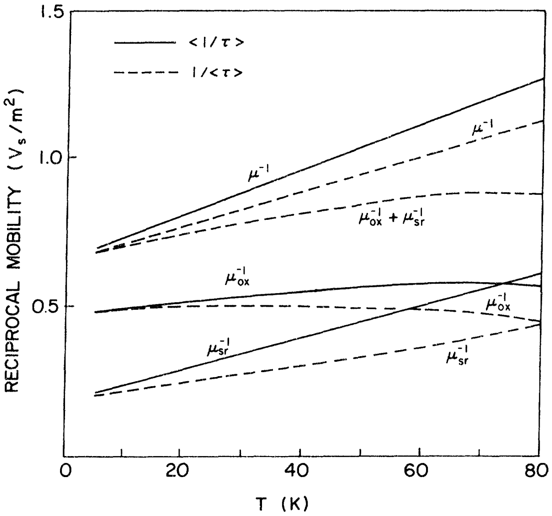

FIG. 1. Temperature dependence of the reciprocal mobility for electrons in Si(100) surface inversion layer. $n=2\times10^{12}$ cm$^{-2}$, $n_{\rm dep}=0.3\times10^{12}$ cm$^{-2}$, $n_I=1.0\times10^{11}$ cm$^{-2}$, $\Delta=6.0\times10^{-8}$ cm, and $d=1.3\times10^{-7}$ cm. The solid curves and the dashed curves are calculated, respectively, according to Eqs. (7) and (11). $\mu_{ox}^{-1}(\mu_{sr}^{-1})$ is the reciprocal mobility due to oxide charges (surface roughness) alone. $\mu^{-1}$ is the reciprocal mobility due to both the scattering mechanisms.

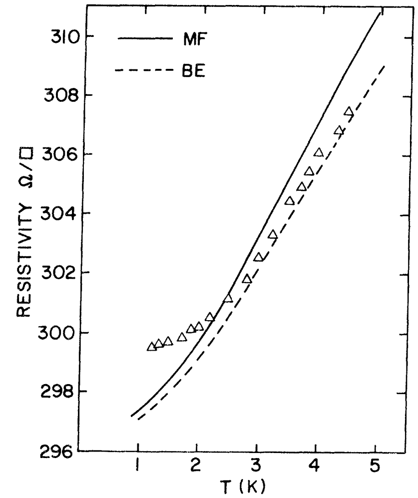

FIG. 2. Resistivity as a function of temperature. The solid curve and the dashed curve are, respectively, obtained from the memory function approach and the Boltzmann equation. The electron density $n=1.3\times10^{12}$ cm$^{-2}$. The small triangles indicate the experimental data of Ref. 4 for sample R3L. All the other parameters used here are identical to those in Fig. 1 or in Ref. 4.

concentration is $n_I=1.0\times10^{11}$ cm$^{-2}$, and the parameters associated with the surface roughness are $\Delta=6.0\times10^{-8}$ cm and $d=1.3\times10^{-7}$ cm. The solid lines are calculated according to Eqs. (4) and (7) which is obtained from the Drude formula [Eq. (3)]. The dashed curves are calculated according to Eqs. (10) and (11) which is obtained from the conductivity by solving the Boltzmann equation [Eq. (8)]. Both of these results show a linear $T$ dependent term in the inverse of the mobilities $\mu^{-1}$ at low temperatures. But the slopes of them are different. It seems that the temperature dependence in $\mu^{-1}$ from the Drude formula is stronger than that from the Boltzmann equation. In Fig. 1, $\mu_{ox}^{-1}$ is entirely due to the scattering of electrons with oxide charges and $\mu_{sr}^{-1}$ is solely from the surface roughness. $\mu^{-1}$ is the reciprocal mobility due to both of the scattering mechanisms. In order to compare with the recent experimental measurements,[4] we also calculated the resistivity for electrons in the (100) surface of Si inversion layer as a function of $T$ for $n=1.3\times10^{12}$ cm$^{-2}$. This is shown in Fig. 2. The small triangles there indicate the experimental data of Ref. 4 for sample R3L. The solid curve is calculated according to the Drude formula or the memory function. The dashed curve is calculated according to the formula obtained from the Boltzmann equation. If we pick the concentration of the oxide charge, $n_I=1.0\times10^{11}$ cm$^{-2}$. The parameters $\Delta$ and $d$ are the same as those in Fig. 1. The values of these parameters have also been used in Refs. 4 and 8. Both of the calculated results show that the resistivity has a linear $T$ dependent term for $T>2.5$ K. This is in agreement with experimental measurements.[4] For $T<2.5$ K, the linear $T$ disappears and a $T^2$ term shows up in the resistivity curves. With the parameters mentioned above, although both of the calculated curves are able to explain the qualitative feature of the experimental data, it seems that the dashed curve obtained from the Boltzmann equation agrees better with measurements.[4] But if the impurity concentration $n_I$ is increased slightly while the surface roughness parameters $\Delta$ and $d$ are decreased; for example, the values of $n_I$, $\Delta$, and $d$ used in Fig. 2 are varied from $1.0\times10^{11}$ cm$^{-2}$, $6.0\times10^{-8}$ cm, and $1.3\times10^{-7}$ cm to $1.05\times10^{11}$ cm$^{-2}$, $5.4\times10^{-8}$ cm, and $1.25\times10^{-7}$ cm, respectively; the slopes of those curves in Fig. 2 will be lowered. The result (solid curve) obtained from the Drude formula will agree better with the experimental data. This is shown in Fig. 3. We can conclude that it is rather difficult to make a decisive comparison between these two approaches with experimental measurements unless the parameters involved with the

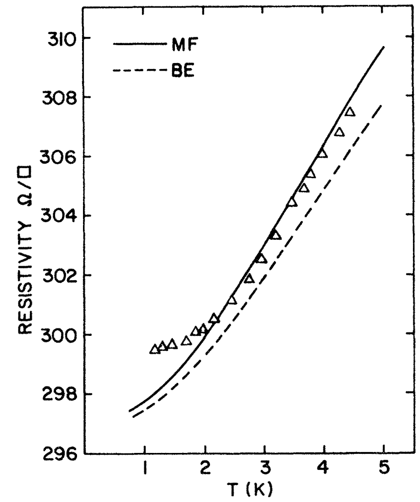

FIG. 3. The resistivity as a funtion of temperature for $n_I = 1.05\times10^{11}$ cm$^{-2}$, $\Delta = 5.4\times10^{-8}$ cm, and $d = 1.25\times10^{-7}$ cm. All other parameters and the representations for notations are identical to those in Fig. 2.

present problem can be determined to high degrees of accuracy.

At this stage it may be interesting to note the reason why the solid curve is always larger than the dashed curve $T\neq 0$. This phenomenon can be understood very easily for $T << E_F$. Since the difference between the solid curve and the dashed curve is proportioned to $\langle 1/\tau\rangle - \langle\tau\rangle^{-1}$, Eqs. (4) and (10) can be expanded up to $T^2$ term. We have

$$\left\langle \frac{1}{\tau} \right\rangle - \langle\tau\rangle^{-1} = \frac{(\pi T)^2}{3} \left[ \frac{1}{\tau^3(E)} \left[ \frac{\partial\tau(E)}{\partial E} \right]^2 \right]_{E=E_F} . \tag{14}$$

If the same set of parameters are used for both methods, the above result shows that the resistivity calculated from the Drude formula is always larger than that from the Boltzmann equation. The difference between $\langle 1/\tau\rangle$ and $\langle\tau\rangle^{-1}$ at finite temperature for a noninteraction electron gas was previously pointed out by Humberman and Chester.[9] It is believed that the Boltzmann equation gives the right result because of the Kubo-Greenwood theorem.[10] However, in the present paper, we have studied the mobility of an interacting electron gas. Not only the difference between $\langle 1/\tau\rangle$ and $\langle\tau\rangle^{-1}$ has been shown to exist in the present case, the actual size of those differences as function of $T$ has also been computed numerically for electrons in Si surface inversion layers.

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