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Y. C. Cheng

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Effect of charge inhomogeneities on silicon surface mobility*

Y. C. Cheng

Bell-Northern Research, Ottawa, Ontario, Canada
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A calculation is presented to estimate the effect on silicon surface mobility of the potential fluctuation due to a random distribution of localized charges near the interface. With a choice of reasonable values for two parameters, the mean–square charge deviation and the correlation length, the theoretical mobility agrees rather well with experiments at low gate voltage and very low temperatures.

In the studies of the physical properties of metal-oxide-semiconductor structures, a uniform distribution for oxide charges as well as for interface states is usually assumed.[1] Recently, it has been suggested[2,3] that these charges are actually randomly distributed rather than having a uniform distribution. The effect of this charge inhomogeneity on surface electrostatics[4] and on the conductance peak[5] of MOS devices has been discussed in the literature. However, the effect of the random distribution of charges on surface mobility has not been investigated. The present work reports some initial effort in this investigation and discusses some preliminary results.

Within the silicon surface region, the equipotential surface is not planar but rather becomes "bumpy" because of the random distribution of both oxide charges and interface states. As a consequence, charge carriers will be scattered by the surface potential fluctuation. This additional scattering mechanism reduces the relaxation time and consequently the mobility of these carriers. A perturbation approach is employed to estimate the scattering effect of the fluctuating potential. The relaxation time is given by

$$\frac{1}{\tau}=\frac{2\pi}{\hbar}\sum_{n'}\frac{A}{(2\pi)^2}\int d^2k'\,(1-\cos\theta)\,|\langle\psi_{n'}|\,\delta u\,|\psi_n\rangle|^2\delta(\epsilon_{n'}-\epsilon_n), \tag{1}$$

where ψ_n, ϵ_n, and k are the wave function, energy, and wave vector of the carriers, respectively, and θ is the angle between the wave vectors k' and k. δu is the deviation in surface potential from a uniform distribution of charges, and is related to the amount of charge deviation $\delta\Omega(R,z)$ via[4]

$$\delta u(R,z)=\frac{2e}{\kappa_{si}}\int d^2Q\,\delta\Omega(Q)\frac{\exp(i\mathbf{Q}\cdot\mathbf{R})\exp(\kappa z)}{\kappa+\gamma Q}, \tag{2}$$

where $\gamma=\kappa_{ox}/\kappa_{si}$ (κ_{ox} is the dielectric constant of oxide and κ_{si} is the dielectric constant of silicon);

$$\kappa=(Q^2+q_0^2)^{1/2},\quad q_0^2=4\pi N_B e^2/\kappa_{si}k_BT;$$

$$\delta\Omega(Q)=(1/A)\int d^2R\,\delta\Omega(R,z)\exp(i\mathbf{Q}\cdot\mathbf{R}). \tag{3}$$

N_B is the dopant concentration, k_B is Boltzmann's constant, and T is the temperature in °K. A is the area of the system perpendicular to the z direction.

In the derivation of Eq. (2), the distribution for the free charge carriers in the surface space-charge region is assumed[4] to have an exponential form, instead of being solved self-consistently by the coupled Poisson and Schroedinger equations.[6] Errors involved in this approximation are not serious as we are only interested in computing the potential deviation rather than the exact energy levels and charge distribution. Furthermore, it should be noted that the deviation in potential given by Eq. (2) may not be the most appropriate to an MOS structure, but it does give a sufficiently correct description of the actual situation and provides a simple expression through which we can estimate the effect of potential fluctuation. Our results should therefore be interpreted within the context of the approximations made in Ref. 4.

In computing the matrix element, the ground-state wave function obtained by Stern and Howard[6] is used and is given by

$$\psi_n=\exp(ik_xx)\exp(ik_yy)(\tfrac{1}{2}b^3)^{1/2}z\exp(-\tfrac{1}{2}bz)$$

and

$$b=[(48\pi e^2m_\perp/\kappa_{si}\hbar^2)(N_B+\tfrac{11}{32}N_{inv})]^{1/3}.$$

It is understood that the wave function is properly normalized and the matrix element is obtained as follows:

$$\begin{aligned}&\langle\psi_{n'}|\,\delta u(R,z)\,|\psi_n\rangle\\&=\frac{2e}{\kappa_{si}}\int d^2Q\frac{\delta\Omega(Q)}{\kappa+\gamma Q}\int\exp[i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{R}]\,d^2R\exp(i\mathbf{Q}\cdot\mathbf{R})\\&\quad\times\int dz\,\tfrac{1}{2}b^3z^2\exp[-(b+\kappa)z]\\&=\frac{4\pi e}{\kappa_{si}}\frac{\delta\Omega(Q)}{\kappa+\gamma|\mathbf{k}'-\mathbf{k}|}\left(\frac{b}{b+\kappa}\right)^3.\end{aligned} \tag{4}$$

By changing the variable from R to $R+R'$, we find

$$\begin{aligned}&|\langle\psi_{n'}|\,\delta u\,|\psi_n\rangle|^2\\&=\left(\frac{4\pi e}{\kappa_{si}}\right)^2\frac{1}{A^2}\int\int d^2R\,d^2R'\,\delta\Omega(R+R')\,\delta\Omega(R')\\&\quad\times\exp(i\mathbf{Q}\cdot\mathbf{R})\left[\frac{1}{\kappa+\gamma Q}\left(\frac{b}{b+\kappa}\right)^3\right]^2.\end{aligned} \tag{5}$$

Now we have to make some approximation to the actual distribution function of the charge deviation $\delta\Omega(R)$. A number of distributions can be used for the charge deviation function. However, as a first attempt we find it convenient and also quite reasonable to assume a Gaussian correlation function for the excess charge fluctuation, i.e.,

$$A^{-1}\int\delta\Omega(R+R')\,\delta\Omega(R')\,d^2R'=N_f^2\exp(-R^2/L^2), \tag{6}$$

where N_f denotes $(\overline{d\Omega^2})^{1/2}$ and is the mean square charge

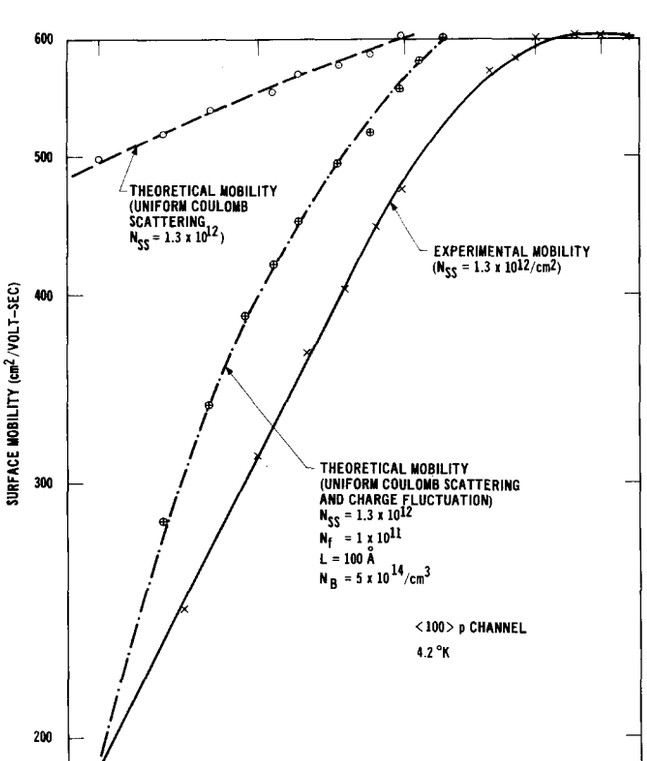

FIG. 1. Comparison of theoretical mobilities with experimental results at 4.2 °K. Experimental surface charge density is $1.3\times10^{12}/\text{cm}^2$.

deviation from the nominal charge density and L is the correlation length which is a measure of average separation of charge bumps; these will be treated later as adjustable parameters in our numerical calculation.

Combining Eqs. (5) and (6), Eq. (1) becomes, after integration over k space,

$$\frac{1}{\tau(k)} = \frac{m_{\parallel} N_f^2 L^2}{\hbar^3}\left(\frac{4\pi e}{\kappa_{si}}\right)^2 \times \int_0^{\pi} d\theta(1-\cos\theta)\exp[-k^2L^2(1-\cos\theta)/2] \times\left[\frac{1}{\kappa+2\gamma k\sin(\theta/2)}\left(\frac{b}{b+\kappa}\right)^3\right]^2, \tag{7}$$

where $\kappa=[2k^2(1-\cos\theta)+q_0^2]^{1/2}$.

It is obvious from this result that the relaxation time is strongly dependent on the wave vector k. The lower the carrier energy (i.e., the smaller k), the stronger is the scattering by the potential fluctuation. For a particular choice of $L=100$ Å, our numerical integration of Eq. (7) shows that $1/\tau(\kappa)$ varies roughly as $k^{-2.8}$ in the small k region which is important for the scattering by surface potential fluctuation. Therefore, it is also apparent that the mobility based on this mechanism will increase very rapidly with the applied surface field.

Figure 1 shows a comparison between the calculated and experimental mobility plotted as a function of the applied gate bias V_g. In order to have a meaningful comparison, we choose a particular sample with a very large amount of surface charge such that its surface mobility at 4.2 °K increases as a function of the applied surface field throughout the major portion of the V_g range. In Eq. (7) N_f is taken to be 10^{11} charges/cm^2, a charge fluctuation which is not unreasonable when the experimental surface charge density is $1.3\times10^{12}/\text{cm}^2$, and L is taken to be 100 Å. Assuming we can treat the Coulomb scattering by potential fluctuation as independent scattering mechanisms, the respective τ's are combined together in the usual manner[7] to yield the resultant mobility for comparison with experiment. At $T=4.2$ °K, $\tau(\kappa)$ is evaluated at the Fermi surface and the Fermi wave vector is related to N_{inv} via $k_f=(2\pi N_{inv}/n_v)^{1/2}$, where n_v is the valley degeneracy. To provide a relative comparison theoretical mobility based on Coulomb scattering[6] without any charge fluctuation is also plotted in Fig. 1.

It is seen that Coulomb scattering without charge fluctuation gives only the correct qualitative behavior. That is, μ increases with V_g, whereas the slope is too small when compared to the experimental result and the magnitude is incorrect, especially at very low V_g. With the inclusion of potential fluctuation due to charge inhomogeneity, the resultant mobility is much closer to the experimental one in both slope and magnitude. The agreement can be improved by a better choice of values for N_f and L. However, we shall not proceed any further in this direction. It seems possible[5] to extract information about N_f from a number of experiments, though reliable ones are not available at the present time. It will be interesting to compare the value for N_f obtained from experimental mobilities using this calculation with values obtained from the other types of experiment, when the latter become available in the near future. Those parametric values we used in computing the theoretical mobility seem to be physically very reasonable. The charge fluctuation corresponds to a 7% deviation in the mean charge density and the magnitude of L corresponds to the average charge separation for our choice of the mean fluctuation charge density.

Our low-temperature measurements give some experimental support to our theoretical model. We found[8] that the slope of the mobility in the low V_g region increases with the surface charge density N_{ss}. It is expected that the amount of charge deviation should increase with N_{ss} so that there is a bigger contribution to scattering by potential fluctuation in samples with larger N_{ss}. Since charge fluctuation gives a steeper mobility vs V_g curve than a uniform charge distribution, samples with large N_{ss} will yield mobility results with larger slope.

It should be remarked here that there exists a similarity between scattering by potential fluctuation due to charge inhomogeneity and scattering due to surface roughness.[9] Both mechanisms introduce perturbations on the equipotential surface in the silicon surface layers. In fact, both have similar dependence on k except that surface roughness scattering has an additional explicit dependence on the applied field which overrides the k dependence and causes the mobility to decrease with increasing V_g instead of increasing.

In summary, we find that scattering by potential fluctuation due to a random distribution of charges is very important especially in the low gate voltage region and at very low temperature. Our model based on this scattering mechanism predicts a surface mobility which is closer to the experimental value than that obtained by the usual Coulomb scattering calculation which assumes a uniform distribution. Furthermore it gives a more realistic dependence on the gate voltage. However, the calculation requires two adjustable parameters, and in the present comparison those values required to give the correct magnitude for mobility are very reasonable figures. Therefore, this scattering mechanism seems to be very promising in explaining the low-temperature low-field-mobility data. However, we will not be satisfied as to the significance of the role that charge inhomogeneity actually plays in determining the low-field transport behavior until charge fluctuation can be measured independently. It is hoped this work will stimulate further effort to study the surface transport problem until it is thoroughly understood.

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