Use of Kubo formalism to study transport beyond the Born approximation: Application to low-temperature transport in Si metal–oxide–semiconductor field-effect transistors

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A formalism is developed to study transport in semiconductor devices under conditions where the Born approximation and independent scattering approximations break down. The approach based on the Kubo formalism is applied to Si metal–oxide–semiconductor field-effect transistors (MOSFETs) where interface roughness effects cause the approximations mentioned above to break down at low temperatures. Results presented are the outcome of a numerical method based on a three-dimensional approach to examine the interface roughness effects on the electronic spectrum as well as on the transport in the MOSFETs. The dependence of mobility on temperature and gate bias are reported and the shortcomings of the Born approximations are outlined. The approach is general and can be applied to problems where scattering is very strong and localization effects are significant, e.g., in amorphous semiconductor devices. © *1998 American Institute of Physics.* [S0003-6951(98)04737-8]

Our understanding of transport in semiconductor devices depends upon the use of the Born approximation and the assumption that various scattering mechanisms are independent. In many problems of interest it is known that the Born approximation is not valid but it is still used because of the complexity of the problem. Examples include transport in metal–oxide–semiconductor field-effect transistors (MOSFETs) at low temperature when a significant fraction of carriers are in the localized bandtail states, transport in clustered alloys, etc. The availability of powerful computers now makes it possible to address the transport problem using more accurate formalisms. The successful implementation of these more accurate formalisms can then allow us to address transport in materials like amorphous silicon, conducting polymers, clustered alloys, etc. In this letter we present results on the use of the Kubo formalism in Si MOSFETs. We examine how interface roughness influences transport as the interface quality degrades.[1–3]

Models based on the Born approximation to study the interface roughness scattering have been used to study mobility in the two-dimensional channel.[4–6] Using island height and lateral extent as fitting parameters, reasonably good agreement with experiments at room temperature[7] has been demonstrated in high-quality MOSFETs. However, at low temperatures it is known that localization effects due to interface roughness are quite important. Thus, mobility increases with temperature instead of decreasing, a sign of hopping conduction.[8–10] A formalism that can address transport in localized and extended states is the Kubo formalism. However, to find the conductivity it is necessary to solve for a three-dimensional Hamiltonian including the interface roughness.

To calculate the electronic spectrum of a two-dimensional electron gas in a MOSFET, two steps have been taken in this letter. First, the potential profile along the direction perpendicular to the Si/SiO_2 interface in a MOS structure is obtained by solving the Schrödinger equation and Poisson equation self-consistently[11] (one-dimensional problem). Then, the potential profile obtained in the one-dimensional problem is used in a three-dimensional Schrödinger equation to yield the electron spectrum. In order to be consistent with the results obtained in the first step, the Fermi level of the MOSFET device is adjusted so that it gives the same occupation number.

The boundary conditions along the *xy* plane (parallel to the interface) are chosen to be periodic in order to calculate the transport quantities. Since we solve for the *electronic levels in the presence of the interface roughness* in the MOS channel, the effect of this roughness on the microscopic and macroscopic properties of the structure can be calculated directly from the electronic spectrum. The Kubo formula[12] for the conductivity of an electron under a small dc field is given by

$$\sigma = \frac{2\pi e^2 \hbar^3 V}{m^{*2}} \int -\frac{\partial f}{\partial E} |D(E)|^2 N^2(E) dE, \tag{1}$$

where the reduced momentum matrix element $D(E,E')$ is expressed as

$$D(E,E') = \int_{E=E'} \psi_E \frac{\partial}{\partial x} \psi_{E'} d\mathbf{r}. \tag{2}$$

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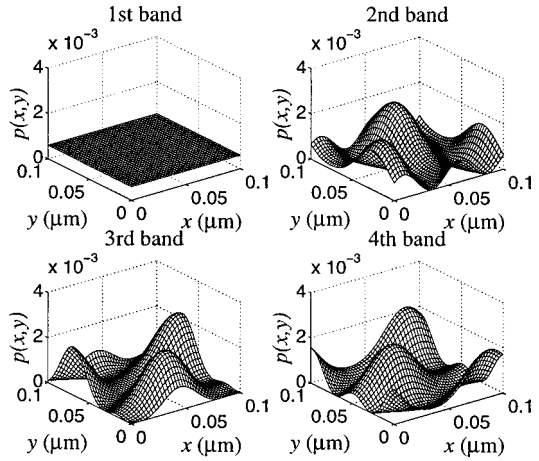


FIG. 1. Electron probability distribution functions $P(x,y)$ for a perfect interface under strong inversion. The corresponding charge density at the interface is $6.7\times10^{12}\,\mathrm{cm}^{-2}$. The wave functions extend to the device (chosen to be 0.1 μm$\times$0.1 μm). The MOSFET studied has 100 Å thick SiO_2 with a p-type substrate doped at $1\times10^{14}\,\mathrm{cm}^{-3}$.The operating temperature is assumed to be 77 K.

Equation (1) will render a conductance for two-dimensional electron gas. Once the conductance is derived, the mobility is readily calculated.

To achieve reasonable results numerically calculated from a discrete electron spectrum due to the finite sample size chosen for study, a Gaussian broadening function is used for both the density of states $N(E)$ and the reduced momentum matrix $D(E)$. The reduced momentum matrix is evaluated by

$$|D|^2_{\mathrm{av}}=\frac{\Sigma_i|\int\psi_{E_i}(\partial/\partial x)\psi_E d^3x|^2 w_\Gamma(E_i,E)}{\Sigma_i w_\Gamma(E_i,E)}, \tag{3}$$

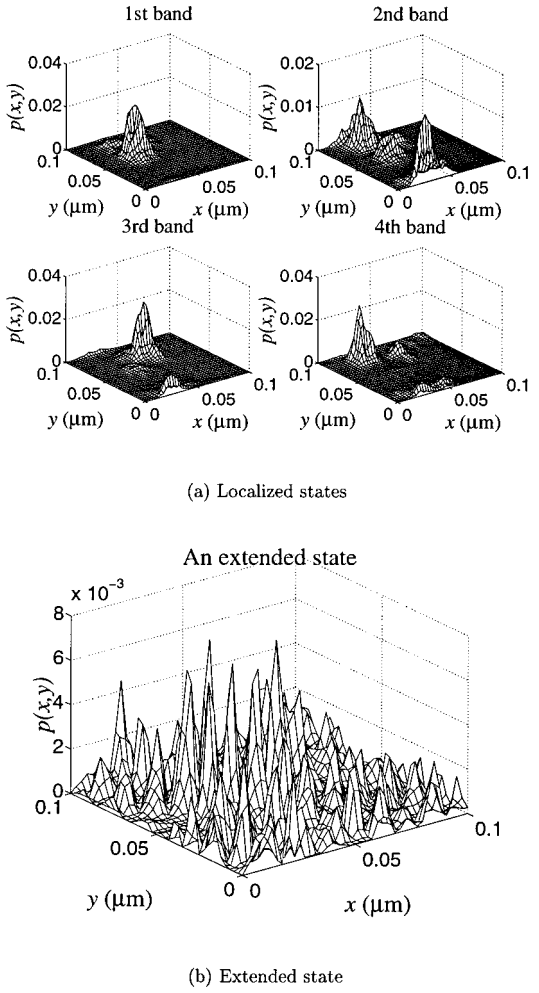
where $w_\Gamma(E_i,E)$ is an integral over the overlapping region between two Gaussian broadening functions centering on energy levels E_i and E, respectively. The quantity Γ is the half width of the broadening functions and represents the lifetime of the corresponding state due to the effects of scatterings (phonons).

Along the z direction the device structure is assumed to be made up of three regions: (i) a region which has perfect silicon dioxide; (ii) a region that has a random distribution of Si and SiO_2 islands; and (iii) a region that has perfect Si. Interface roughness is introduced by randomly placing islands on the intermixed region of the MOS structure with the island size given by

$$\Delta L_x=25\,\text{Å},\quad \Delta L_y=25\,\text{Å},\quad \Delta L_z=5,10\,\text{Å}. \tag{4}$$

The Schrödinger equation is solved by the matrix method. The results shown in this section are for a MOSFET structure with 100 Å oxide thickness and a background p-type doping of $1\times10^{14}\,\mathrm{cm}^{-3}$.

In Figs. 1 and 2 we show the electron probability distribution functions $P(x,y)$ on the xy plane in a MOSFET with a perfect interface and a rough interface, respectively. From Fig. 1, one can see that the electron wave functions for a perfect interface extend over the entire device and have a peak amplitude of 0.0024 corresponding to the normalization in the 1000 Å$\times$1000 Å xy plane. However, for the imperfect interface the eigenstates are quite different. We see from Fig. 2 that the low-lying states are strongly localized (e.g., the peak amplitude of the first state is 0.022, one order of magnitude larger than the case for the perfect interface). The lateral spread of these states is 200–250 Å. The position of these low-lying states will change if we change the random sequence of the disorder, but the localization length is in the same range. This suggests that to study transport in such a system the use of the Born approximation is invalid. We also see that as we go to higher-energy states, the states become extended and are spread over the entire structure.



(a) Localized states

(b) Extended state

FIG. 2. Electron probability distribution functions $P(x,y)$ for the same bias as Fig. 1 but with an interface roughness (height: 5 Å; lateral extension: 25 Å). The low-lying states are clearly localized but the excited states are extended.

Next, we report results for the mobility in the channel using the Kubo formalism. From our discussion of localization we can see that the imperfect interface mobility will be very small unless the electrons can couple from one state to another by other scattering processes such as phonons. Thus, for the imperfect interface case we expect that as the broadening parameter Γ increases, mobility will initially increase. For the case of the perfect interface, on the other hand, as Γ increases the mobility should decrease.

For the MOSFET at 77 K, acoustic phonon scattering is expected to be the dominant scattering mechanism. Using the acoustic phonon scattering rates for the Si inversion layer we find that Γ is expected to be 0.34 meV.

In Fig. 3 we show the calculated relationship between

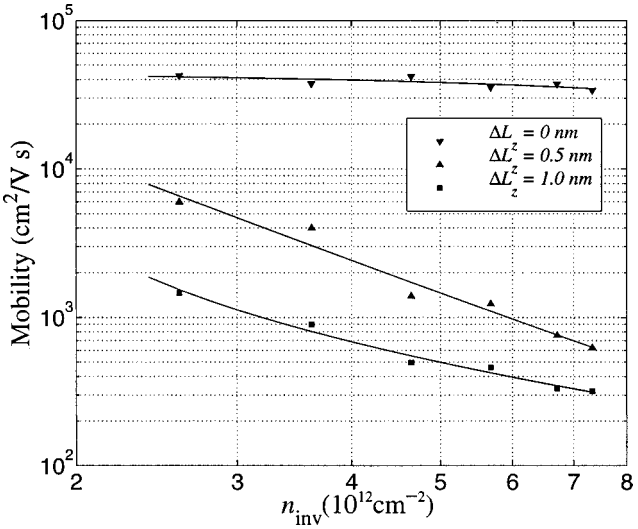


FIG. 3. Electron mobility as a function of sheet charge density, n_{inv} for (a) $\Delta L_z = 0$ nm, (b) $\Delta L_z = 0.5$ nm, and (c) $\Delta L_z = 1.0$ nm. The half width of the Gaussian broadening function, $\Gamma = 0.34$ meV corresponds to the phonon scattering rate at 77 K.

the mobility and sheet charge density in the channel. Results are shown for the perfect interface and for imperfect interfaces with $\Delta L_z = 5$ Å and $\Delta L_z = 10$ Å. From Fig. 3, one can see that the mobility for the device with the perfect interface is almost independent of the sheet charge density. This value agrees quite well with the mobility calculated using the Born approximation and acoustic phonon scattering. For the device with the interface roughness, the mobility is found to have a strong dependence on the sheet charge density. This is to be expected since as the sheet charge density is increased the electron charge is pushed closer to the interface. Use of the Born approximation shows that the mobility should be inversely proportional to the square of the sheet charge. For the case with $\Delta L_z = 5$ Å, we find that the mobility is proportional to $n_{\mathrm{inv}}^{-2.2}$, a slight deviation from the model based on the Born approximation. For the case of $\Delta L_z = 10$ Å, where localization effects are very strong, there is no simple relation between the mobility and the sheet charge density.

In Fig. 4 we show the mobility as a function of temperature from 30 to 110 K for $\Delta L_z = 5$ Å. The corresponding sheet charge density is $2.4 \times 10^{12}\,\mathrm{cm}^{-2}$. Figure 4 shows that *the mobility increases as the temperature increases at low temperature*. As discussed earlier, this is attributed to the importance of phonon-assisted hopping in this regime. It is not possible to understand this regime using the Born approximation and the standard transport theory where scattering mechanisms are independent. However, as the temperature increases to high values, the mobility starts to decrease, as shown in Fig. 4. This is primarily due to the increasing phonon scattering as the temperature increases. This characterization of electron mobility has been verified in the experiment.[13]

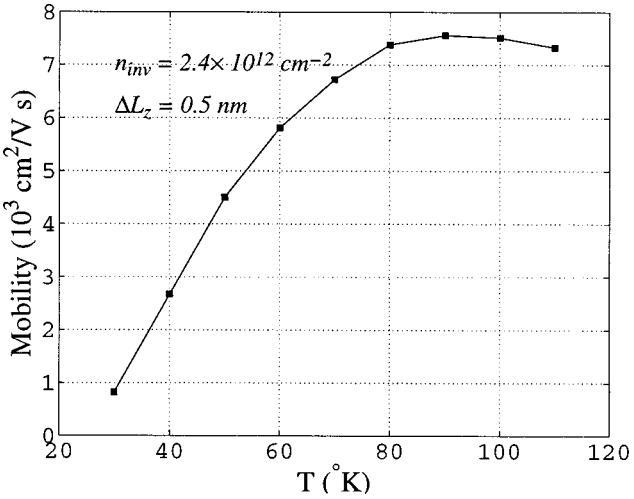


FIG. 4. Electron mobility as a function of temperature *T*. The corresponding sheet charge density is $2.4 \times 10^{12}\,\mathrm{cm}^{-2}$.

In summary, we have developed a numerical formalism to examine the effects of interface roughness in MOSFETs. We see that at low temperatures, under strong inversion conditions, to study transport, the use of the Born approximation is invalid due to the strong localization of the low-lying states. However, when the carrier density is small (the channel is relatively wide and the electron wave functions do not overlap as strongly with the interface region), the use of the Born approximation is valid. Our model allows us to examine the effect of gate bias and the degree of interface roughness on transport properties. At low temperature the mobility increases with temperature, which cannot be understood by the model based on the Born approximation. The application of the Kubo formalism shows this increase, which is consistent with experiments.

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