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Calculated transport properties of ultrasubmicrometer quasi-one-dimensional inversion lines

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We calculate low-temperature dc transport properties of a quasi-one-dimensional electron system as occurring, for example, in ultranarrow inversion layers. Density of states and conductivity are theoretically calculated in realistic structures as a function of the chemical potential. As the chemical potential sweeps through quantized one-dimensional subband states, well-defined oscillatory structure is seen in the density of states and in the conductivity, provided the level broadening and temperature are low. Detailed numerical results and a qualitative comparison with existing experimental data are given.

Much attention has recently been focused on quasi-one-dimensional (1D) electronic states in very narrow semiconductor microstructures where electronic motion is quantum-mechanically confined in two directions (while being free in the third dimension along which 1D transport can occur). Advances in lithographic and molecular-beam epitaxy techniques make it likely that the study of quasi-one-dimensional electron systems will grow rapidly in the near future. Most of the recent experimental[1] and theoretical[2] work has concentrated on strong and weak localization properties of these ultranarrow structures. In particular, lack of ensemble averaging in a single small 1D chain leads to significant resistance fluctuations in the strong localization limit.[3] Such strong fluctuations (as a function of the chemical potential) make it impossible to observe quantum-mechanical 1D confinement effects on transport properties of a *single* 1D system. However, Warren *et al.* have recently argued[4] (and we have explicitly verified[5] this contention via direct numerical simulation as shown in Fig. 4 of this paper) that *ensemble-averaged* 1D transport behavior can be observed by having a large number (~ 250 in the actual experiment of Ref. 4) of parallel and identical 1D channels (which do not interact with each other, i.e., lateral electronic hopping is not allowed), so that the net conductance is obtained by summing the conductances of these lines.

In this Rapid Communication we calculate Drude transport properties of quasi-1D electron systems as occurring in very narrow silicon inversion layer channels. We ignore all aspects of localization and conductance fluctuation physics uncritically in this paper (except for what we show in Fig. 4). Our motivation is partly to carry out a calculation which can be compared directly to the published results of Warren *et al.*,[4] and partly to establish criteria under which 1D quantum confinement effects are observable in transport properties of real systems. Our calculation of conventional transport properties of these 1D systems take into account all the *essential* aspects of the actual physical situation. We include in the theory 1D quantization, intersubband scattering, realistic screening, finite level broadening, and finite temperature effects. There exists in the literature earlier work[6] on the calculation of transport properties of 1D quantum wire structures using simpler approximations. To the best of our knowledge, transport in the multisubband 1D situation treated in this paper has never before been dealt with, even though there has been some effort[7] in the corresponding 2D systems.

Our theory is a perturbative theory in the leading-order impurity density. The most important feature of the theory is self-consistency in the sense that the electronic Green's functions entering calculations are all dressed by the impurity scattering diagrams and, hence, the diagrams must be computed self-consistently. Similar self-consistent calculations have also been successfully used in other situations involving strong divergences in the bare one-electron spectral properties, such as a two-dimensional system in the presence of a strong external magnetic field. Calculational details of our theory will be given elsewhere.

Our model is that of electrons confined in two (y and z) spatial dimensions described by single-particle wave functions $\psi(\mathbf{r}) \sim e^{ikx}\phi_n(y)\xi_i(z)$, where k is the free 1D "wave vector" in the x direction and $\phi_n(y)$, $\xi_i(z)$ are the confining wave functions for the nth and the ith subbands, respectively, for the quantized motion along y and z directions. This separation of variables turns out to be a fairly good approximation[8] for the electronic structure of the actual systems of interest[4] to us. It also turns out that the confinement in the y direction (parallel to the Si-SiO_2 interface) is much weaker than the perpendicular confinement in the z direction, so that it is not a bad approximation to take $|\xi_0(z)|^2 \sim \delta(z)$—the actual experimental situation is always such that only the ground ($i=0$) subband of z motion is occupied by electrons. For lateral confinement along the y direction we have chosen a "particle-in-a-box-type" rectangular potential well confinement (from which we have the subband energy $E_n \propto n^2$), and also a "harmonic-oscillator-like" parabolic well confinement (from which we get $E_n \propto n$). Detailed self-consistent numerical work[8] by Laux and Stern shows that the actual confining potential is somewhat in between. In view of uncertainties in the experimental geometry and in the various parameters entering the theory, we feel that either one of these two model potentials is a reasonable approximation to the real 1D system

and, fortunately, our qualitative results are the same in both models.

Since at low temperatures (<10 K) charged impurity scattering is known to be the most important resistive mechanism in silicon inversion layers, we neglect all other scattering mechanisms. Also, the actual random impurity distribution is not well known, and so we choose the random impurity distribution to be uniform in the channel, with an average impurity density N_i.

We start by calculating the density of states $D(E)$ of our model 1D system by first obtaining the impurity-induced level broadening. The level broadening Γ_n is calculated by solving numerically the self-consistent Born approximation for electron-impurity self-energy which should be adequate for low-impurity concentration. The calculation of the self-energy is simplified by noting that the calculated *screened* Coulomb interaction is only weakly dependent on the 1D wave vector in view of the strong screening[9] in the system. The level broadening is found to be approximately

$$\Gamma \approx 28.4\alpha^{4/3}(N_i/N_l)^{2/3}\ \text{meV}\ ,$$

where N_i, and N_l are the effective 1D impurity and electron densities measured in cm^{-1}, and α sets the scale of the typical electron-impurity interaction and is of order 0.1. Thus, for $N_i/N_l=0.1$ one gets $\Gamma\approx 0.4$ meV which should be compared with 2 meV as the energy separation between the ground and the first excited subbands for an infinite rectangular potential well with width $W=500$ Å in the y direction. This corresponds roughly to a mobility of 10000 $\text{cm}^2/\text{V sec}$. Our realistic self-consistent Born approximation calculation of level broadening shows that the broadening Γ_n for our model system depends only weakly on the 1D subband index n (for the low-lying subbands) and, therefore, in Fig. 1 we show our calculated 1D density of states for several different values of the broadening Γ assumed to be a constant for the system. We choose parameters to correspond to the actual experimental system of Ref. 4. In Fig. 1 we show the calculated density of states $D(E_F)$ as a function of the Fermi energy for three values of the broadening $\Gamma=0.15$, 0.38, and 1.52 meV which correspond approximately to mobility values $\mu=20000$, 8000, and 2000 $\text{cm}^2/\text{V sec}$, respectively. The system width is taken to be 500 Å which for our model infinite square-well potential gives $E_n=0.79n^2$ meV, so that $E_2-E_1\approx 2$ meV. Our results [see Figs. 4(b) and 4(c)] are very similar for a parabolic well confinement. In Fig. 2, we show our calculated conductivity σ_{xx} as a function of the chemical potential for different values of broadening (corresponding to Fig. 1) and two different temperatures ($T=1.2$ and 10 K). We use Kubo formula and diagrammatic perturbation theory to calculate σ_{xx}. The message from Figs. 1 and 2 is that at low temperature (~ 1.2 K) and low broadening ($\mu\sim 20000$ $\text{cm}^2/\text{V sec}$) one may be able to see conductivity oscillations in the current-voltage characteristics associated with structure arising from 1D confinement. However, even at moderately low temperature (~ 10 K) these structures are washed out for a 500-Å-wide channel. Our empirical finding is that $\Gamma+k_BT$ should be less than $\Delta E/2$ for 1D confinement effects to be observable. These results agree with the reported findings in Ref. 4, and support the view that the structure observed there is associated with 1D confinement effects.

Above results based on a short-range intrasubband impurity scattering model (which we have explicitly verified to be fairly well valid by doing realistic calculations with

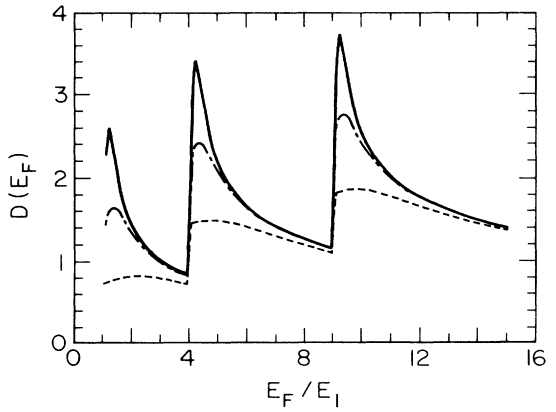

FIG. 1. Impurity-broadened density of states $D(E_F)$ in a model 1D system (infinite square-well confinement with width $=500$ Å) for three different values of the level broadening $\Gamma=0.15$ (solid line), 0.38 (dash-dotted line), 1.52 (dashed line) meV. The Fermi energy is measured in the units of the ground subband bottom $E_1\simeq 0.79$ meV.

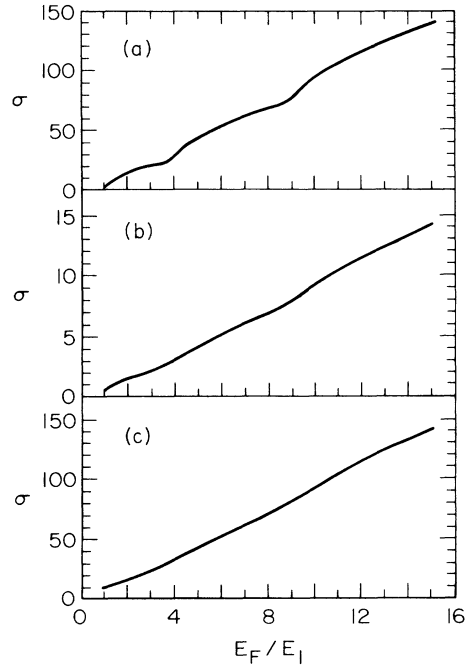

FIG. 2. Calculated conductivity in the 1D system corresponding to Fig. 1 as a function of E_F/E_1 for different values of level broadening (Γ) and temperature (T): (a) $\Gamma=0.15$ meV and $T=1.2$ K, (b) $\Gamma=1.52$ meV and $T=1.2$ K, (c) $\Gamma=0.15$ meV and $T=10$ K. Only intrasubband scattering (due to short-range scatterers) is included. Same absolute units are used in (a)–(c).

screened[9] Coulomb potential as explained earlier) bring out most of the essential physics of 1D transport, except for the very important issue of intersubband scattering which we consider next. The increase in the conductivity seen in Fig. 2 as each 1D subband starts getting populated is due to the peak in the density of states associated with the bottom of each 1D subband. However, in the presence of intersubband scattering there will be substantial reduction in mobility as each new 1D subband is populated due to enhanced scattering between subbands. In fact, the broadening $\Gamma(E_F)$ due to intersubband scattering diverges at $E_F = E_n$ in the ideal non-self-consistent situation due to the singular 1D density of states at the band bottoms. Thus the transport calculation involving intersubband scattering must necessarily be self-consistent, which complicates the theory considerably. We have carried out such a self-consistent transport calculation using the Kubo formula. Our calculated results for the conductivity including intersubband scattering effects are shown in Fig. 3. In Fig. 3(a) we show results of a multisubband transport calculation at $T=0$, using the Kubo formula with and without any self-consistency. In the non-self-consistent case, conductivity vanishes at the bottom of each subband because of enhanced intersubband scattering. In Fig. 3(b) we show the self-consistent *finite-temperature* Kubo formula results. Self-consistency gives rise to finite density of states at the band bottom so that the conductivity does not drop to zero at the bottom of each 1D subband. These conductivity results are obtained by assuming the screened impurity scattering to be short ranged with its strength calculated from the averaged screened Coulomb potential. This approximation is very good for our system in view of strong screening[9] in 1D. We have also carried out a multisubband Boltzmann equation[10] calculation of conductivity using realistic screened[9] Coulomb impurity potential. This calculation is very tedious and completely justifies our Kubo formula results based on the short-range model shown in Fig. 3.

Before concluding we provide a justification of our model (introduced originally in Ref. 4) by showing in Fig. 4 that conductance fluctuations[1-3,5] inherent in small structures are indeed averaged out when a large number of parallel inversion lines are used. One can see from Fig.

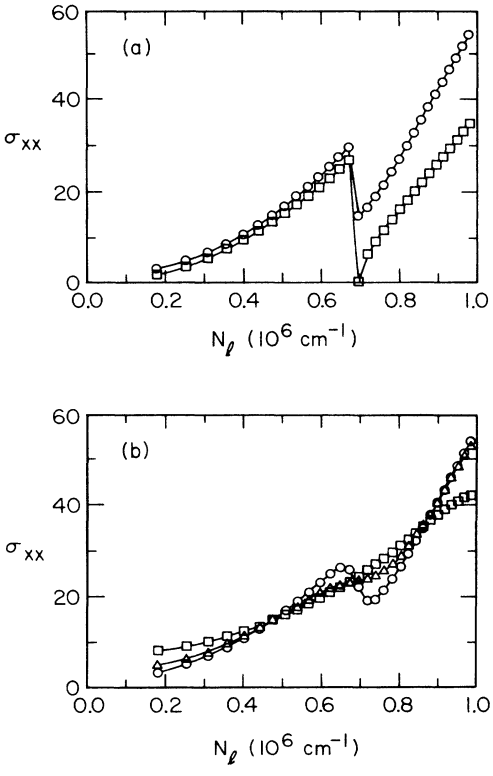

FIG. 3. Calculated conductivity as a function of 1D electron density for the system corresponding to Fig. 1 with $N_i = 1\times10^{11}$ cm^{-2} (distributed uniformly in the channel) including intra- and intersubband impurity scattering. (a) $T=0$ with non-self-consistent (open squares) and self-consistent (open circles) calculations; (b) self-consistent results for $T=1.2$ K (open circles), 4.2 K (open triangles), and 10 K (open squares). Same absolute units are used in all the figures.

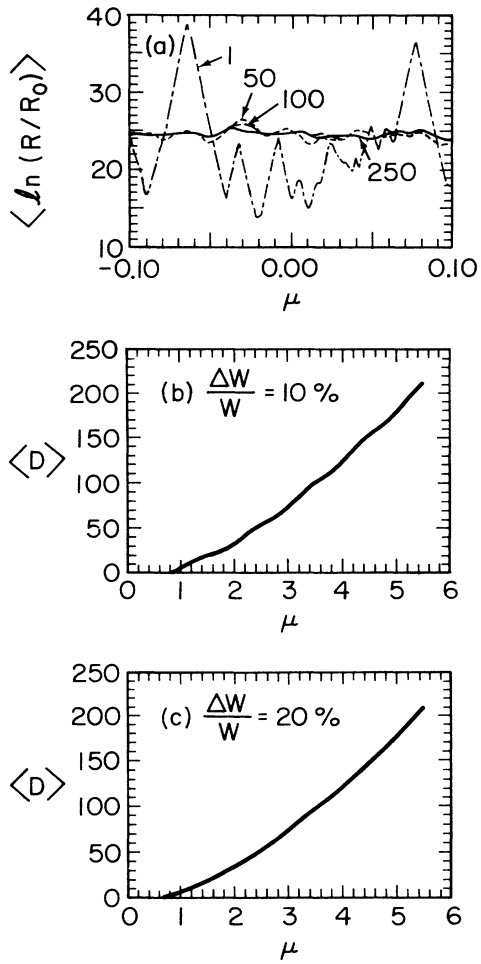

FIG. 4. (a) Calculated average fluctuating resistance $\langle \ln R \rangle$ in a *finite* 1D chain as a function of the chemical potential for various numbers of parallel inversion lines as noted (see Refs. 3 and 5), (b) calculated conductivity D for 250 parallel inversion lines (for parabolic potential confinement) with width fluctuations of 10%, and (c) of 20%. [$\Gamma/E_1 = 0.1$ for (b) and (c).]

4(a) that the resistance fluctuations are substantially suppressed by having a number of parallel 1D channels —in particular, for 250 inversion lines (as used in Ref. 4) fluctuation effects are negligible. On the other hand, quantum confinement effects are much more resilient, as can be seen from Figs. 4(b) and 4(c), where we show the averaged conductivity (using parabolic harmonic oscillator confinement in this case) for a system of 250 parallel inversion lines with substantial width fluctuations. One can see that even with width fluctuations as large as 10%–15% one can observe 1D confinement effects.

In conclusion, we have carried out density of states and transport calculation in model (infinite square-well—and parabolic—potential confinement) 1D systems including thermal and collisional broadening effects. We obtain the density of states in a self-consistent Born approximation and the conductivity using the self-consistent Kubo formula (and coupled Boltzmann equation approach). We find the short-range scattering model to be a good approximation due to strong screening in the system. We find that unlike higher-dimensional systems, self-consistency in the calculation of conductivity is absolutely essential in 1D systems in the presence of intersubband scattering. Our calculated results are in qualitative agreement with the data of Warren *et al.* and show that structures due to 1D quantization may be observable in transport characteristics of very narrow inversion layers, provided the temperature and the impurity content of the system are low.

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