Interaction-Induced Transition at Low Densities in Silicon Inversion Layer

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Intravalley exchange and correlation are found to induce a first-order transition at low densities in the inversion layer, lowering the valley degeneracy. For the n channel on Si(100) surface, the reduction from two valleys to one occurs roughly below 3×10^{11} cm^{-2}. The one-valley phase with domain structure yields activated conductivity and other observed low-density behavior.

Electrons confined to the semiconductor-insulator interface by an electric field form a quasi-two-dimensional electron system. In the case of valley degeneracy [e.g., twofold in Si(100) electron inversion inversion layer], the valleys are assumed to be equally occupied.[1] This mode of population tends to minimize the kinetic energy. On the other hand, the (negative) exchange and correlation energy will be lowered if the electrons are confiend to one valley. Thus, at high densities, where the kinetic energy dominates, the valleys will be equally populated, whereas at low densities, because of the domination of the exchange and correlation energy, fewer valleys will be occupied [one valley in Si(100)].

Unlike Kelly and Falicov,[2] we consider only direct electron-electron interaction and exclude intervalley exchange as being small. Thus, we cannot address ourselves to the controversial problem of valley degeneracy in the normal density range of the electron inversion layers on Si(111) and Si(110) surfaces.[3] Instead, we focus on the consequences at low densities, and, for simplicity, present our arguments in terms of the electron inversion layer on Si(100) surface. At sufficiently low densities ($<10^{12}$ cm^{-2}), either valley (but not both) is occupied and the other, unoccupied valley is caused to have higher energy. We postulate the formation of domains of single-valley occupation at the low-density phase. This model leads to activated conductivity, Hall effect, and Shubnikov–de Haas oscillations in qualitative agreement with observation.

The activated conductivity behavior has led to the suggestion of Mott-Anderson localization.[4] Its inability to account for the observed Hall coefficient has led to the advocation of a pinned Wigner lattice.[5] While one of these possibilities will eventually happen at low densities or higher impurity concentrations, we suggest that the existence of an intermediate phase of singly occupied valley could explain most of the present observations.

The exchange and correlation effects are calculated in the density-functional formalism.[6,7] We include both intravalley and intervalley terms of the Coulomb interaction between electrons, but exclude scatterings of an electron from one valley to another. The functional form is analogous to the spin-density functional.[8] Hence, the physical reason for the occurrence of the single-valley phase is analogous to the ferromagnetic case.[9] For simplicity, we assume equal spin population within a valley.[10] The critical density N_c is dependent on the depletion density N_{dep} ($N_c = 2.3$ and 2.9×10^{11} cm^{-2} for $N_{\mathrm{dep}}=1$ and 3.6×10^{11} cm^{-2}, respectively). Above N_c, the two valleys are equally occupied. At N_c, there is a first-order phase transition and one valley is raised in energy and completely emptied out. Figure 1 shows the den-

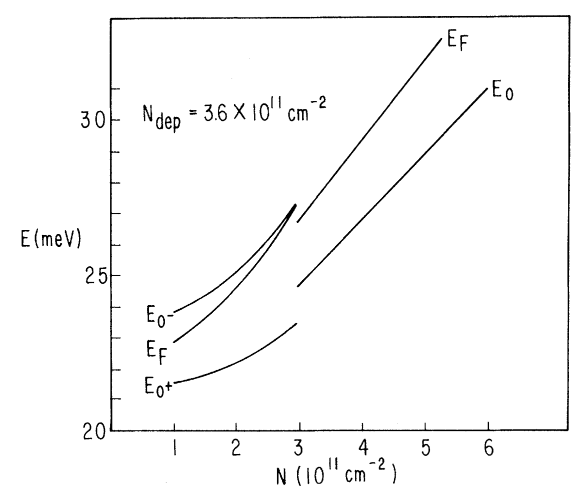

FIG. 1. Results of the density-functional calculation for the lowest subband energy vs density N. At N_c = 2.9 $\times 10^{11}$ cm^{-2}, there is a first-order phase transition which causes a change in the valley degeneracy.

sity dependence of the bottom of the lowest split subbands and the Fermi level.

As the density of the inversion layer is lowered past N_c, an activation energy of the order of 1 meV per electron is needed to empty the electrons from one valley to the other. Therefore, the electrons from each valley group together spatially to form domains in which one valley or the other (but not both) is lower in energy and thus occupied. The domain wall is similar to the Bloch wall in a ferromagnet, being the transition region where the electron density of one valley decreases to zero and where that of the other valley increases from zero to the full value. The domain-wall energy, estimated in the same way as the surface energy of the electron-hole drop,[11] is of the order 10^{-6} eV/Å. The domains form a metastable state provided that the cost in wall energy is small compared with the activation energy. If the wall energy is, say, one-tenth the activation energy, it yields domain size of the order 10^3 Å. The domain walls also tend to be pinned at defects where either the high-density phase is favored or the two valleys are connected by scattering.

The domain structure of the low-density phase gives rise to activated conductivity. Label type A the domain in which $+k_0$ valley is lower in energy and occupied, k_0 being the conduction-band-edge wave vector, and in which $-k_0$ valley is higher in energy and unoccupied. Label type B the domain in which the roles of $\pm k_0$ valleys are reversed. In the absence of intervalley scatterings, an electron in the $+k_0$ valley is free to conduct in domain A, but cannot go across domain B unless it is thermally activated with an energy greater than $W(N)$, the energy difference between the bottom of the $+k_0$ valley subband in domain B and the Fermi level. The calculation of the conductivity becomes a percolation problem. For the $+k_0$ valley electrons, domain A has conductivity σ_1, say, and domain B has conductivity σ_2, so that

$$\sigma_2 \simeq (k_B T/E_F)\sigma_1 e^{-W(N)/k_B T}. \quad (1)$$

All the electrons are assumed to have the same mobility and the post factor multiplying σ_1 is the number of thermally excited electrons. For $-k_0$ electrons, domain A has conductivity σ_2 and domain B has conductivity σ_1. The effective-medium theory, which provides a good approximation for the usual two-dimensional system of one type of electrons in two types of conducting domains,[12] is extended for the two types of electrons. By neglecting intervalley scatterings, each type of electron follows its own equation of continuity. Therefore, for a given configuration of the domains, each valley of electrons experiences a different effective force which is partly due to the common electric field and partly due to the density gradient from the same valley which is calculated in the effective-medium approximation.

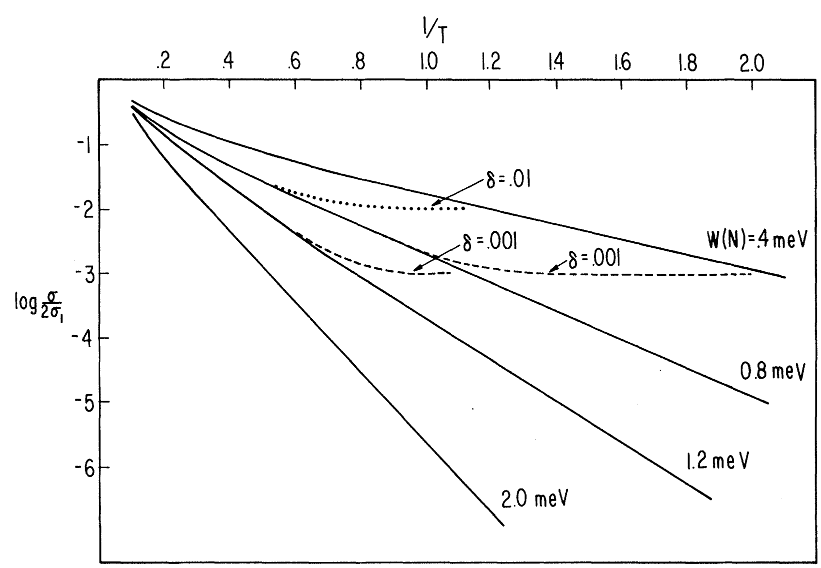

FIG. 2. Plot of the conductivity vs inverse temperature [Eq. (2)] for N in the activated region. $W(N)$ is the activation energy in Eq. (1). The solid curves are for $p = p_c = 0.5$. The dashed curves are for small deviations, $\delta = 0.001$, from p_c. The dotted curve is for $\delta = 0.01$. Note the saturation of the conductivity at low temperature.

The effective conductivity is given by

$$\sigma = [(1-2p)^2(\sigma_1-\sigma_2)^2 + 4\sigma_1\sigma_2]^{1/2}, \tag{2}$$

p being the fraction of domains of type A. Were there only one valley, $p=\frac{1}{2}$ would be the critical fraction for the conductor-insulator transition. With two valleys, the conductivity is symmetric about $p=\frac{1}{2}$, where it is activated. For p close to $\frac{1}{2}$, for a large range of temperature, it is close to $\exp\{-W(N)/2k_BT\}$ dependence. The apparent activation energy in the conductivity measurement is half the activation energy $W(N)$. At the lowest temperatures it shows saturation as was found by Sjöstrand, Cole, and Stiles[13] (see Fig. 2). The range of $W(N)$, obtained from Fig. 1, is in rough agreement with various measurements.[13] The sample dependence[14] may be due to a small variation in the domain fraction p.

Changing the substrate bias to increase $N_{\rm dep}$ will increase the activation energy at a given density in our model, contrary to Fowler's observation,[15] although the experimental picture seems unclear.[14] The substrate bias may change the domain fraction p, whose effect on conductivity is more complex. The frequency dependence of the conductivity from our model of the low-density phase is in qualitative agreement with the observations of Allen *et al.*[16]

The Hall coefficient in low field is calculated with a two-band model for the two types of electrons in the effective-medium theory.[12,17] The assumption of the same mobility μ for all the electrons leads to

$$R = \mu/(\sigma_1+\sigma_2). \tag{3}$$

Thus, R is a measure of the total density,[18] and the Hall mobility is activated. Note that the denominator in (3) is not the dc conductivity given by (2). The result is easily understood in terms of a simple two-band two-domain model, taking into account the key fact that the density is uniform. This is in agreement with the Hall measurement by Thompson.[19]

On reducing the density across the phase transition, the number of occupied Landau levels increases since the electrons are then concentrated in one valley. Shubnikov–de Haas oscillations at low densities should show extra periods. A qualitative picture is shown in Fig. 3. We believe that one extra period was observed by Lakhani and Stiles.[20] The appearance of a low-density peak in the transconductance on increasing substrate bias can be explained in terms of the increase of the critical density and hence the appearance of the

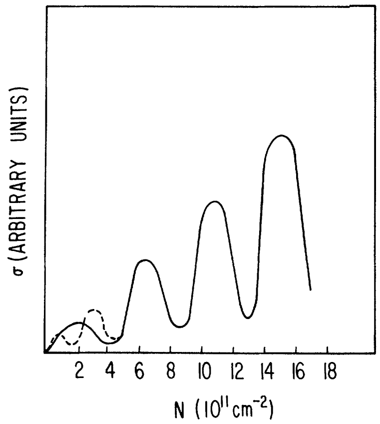

FIG. 3. Sketch of Shubnikov–de Haas oscillations as a function of N for a magnetic field of 4.4 T. The solid line is the result if no transition occurs. The dashed line shows what happens if the transition occurs at $N_c \cong 4\times10^{11}$ cm^{-2}.

single-valley phase. Otherwise, this peak position as a function of the density does not match the other peaks.

In conclusion, we have attempted to show that an exchange-correlation–induced transition offers a reasonable alternative description of the properties of the electron inversion layers of Si at low densities. While the unequal–valley-population case cannot be applied to single-valley space-charge layers, the unequal–spin-population case can be used to explain the low-density behavior, e.g., the activated conductivity.[10]

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Evidence Against Solitons in Polyacetylene: Magnetic Measurements

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EPR and dc conductivity measurements in pristine and acceptor-doped *cis*-$(CH)_x$ and pristine *trans*-$(CH)_x$ are reported. At dopant concentrations of 0.7% and 0.9% AsF_5, the *cis* isomer shows a Pauli susceptibility and a conductivity that seem to arise from randomly distributed, highly conducting regions—a sign of dopant aggregation. There in no need to invoke charged solitons. Comparison with previous experimental results suggests that they do not support the existence of charged solitons in the doped *trans* isomer; neutral solitons in the undoped *trans* isomer are also questioned.

Doped polyacetylene $[(CH)_x]$ has recently become a subject of considerable interest. Its electronic properties are roughly similar to those of a simple classical semiconductor: the dc conductivity σ increases rapidly with concentration at low dopant levels and shows an insulator-metal transition at some higher level.[1,2] The magnetic properties that have been reported[3,4] contrast remarkably with these. First, the spin susceptibility χ that was observed in pristine *trans*-$(CH)_x$ was Curie-like. Furthermore, χ did not appear to increase on light acceptor doping with AsF_5,[4] which increased σ by a factor of 10^5,[1] nor did it change on compensation with NH_3,[3] which decreased σ by a factor of 10^4.[1] This suggested[4] that the charge carriers in lightly doped material carry no spin. Second, although the spin concentration in pristine *trans*-$(CH)_x$ was estimated from χ to be only one spin per 3000 carbon atoms, the EPR absorption line was Lorentzian with a width of 1.43 G at 296 K. This suggested[3] that the spins are mobile.

Noting that there are two equivalent dimerizations for a *trans*-$(CH)_x$ molecule, differing only by the interchange of the shorter (double) and longer (single) bonds, Goldberg *et al.*[3] suggested that domains of both kinds could coexist in the polymeric chain and that the resulting domain walls (mathematically akin to "solitons" or