Mott-Anderson Localization in the Two-Dimensional Band Tail of Si Inversion Layers

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Experimental evidence for a transition from localized to extended states in a two-dimensional band tail is obtained by measuring the conductivity in n- and p-type inversion layers in Si as a function of electron density and temperature (4.2 to 0.4°K). A transition from metallic to thermally activated conductivity is observed as a function of electron density, while the temperature dependence at electron densities below the transition shows both thermally activated nearest-neighbor hopping and variable-range hopping as proposed by Mott.

Present technology for fabricating Si MOSFETs (metal-oxide-semiconductor field-effect transistors) has made the Si inversion layer a unique model system for the study of electronic processes in a two-dimensional (2D) electron gas.[1] Its carrier density can be varied by several orders of magnitude simply by varying the voltage to the metal gate. Fang and Fowler[2] first made an extensive study of the transport properties of n-type Si inversion layers at temperatures from 300 to 4.2°K. They discovered that at low temperatures the dc conductivity is thermally activated at low surface-carrier concentration n_s and metallic at high n_s. Recently, Mott[3] has suggested that these low-temperature results may demonstrate the existence of a mobility edge in the band-tail states of the inversion layer separating the localized states from the extended states.[4] The potential fluctuations, which create this tail of localized states in the bottom of the 2D sub-band, arise from interface roughness and from charges in the oxide and at the interface. Stern[5] has examined the published experimental data which can be interpreted as supporting this mobility-edge model and has pointed out that, although these data are reasonably explained by a mobility edge, they do not exclude alternative explanations. For example, the low-temperature results of Fang and Fowler have also been explained by electron freezeout on bound states in the inversion layer arising from positively charged interface centers.[6] Thus, although it has been appreciated for some time that the threshold for metallic conductivity in these systems occurs above the charging threshold, the exact nature of the localization near the conduction threshold has not been elucidated. In the following we demonstrate that Mott's model for localization by potential fluctuations in a band tail may be applicable to these systems by making measurements of the channel conductance as a funtion of temperature.

We have studied the temperature dependence of the dc resistivity of p-type as well as n-type Si inversion layers from 4.2 to 0.4°K and obtained a number of results which support Mott's[3] mobility-edge model. First, we have observed the transition from the metallic conduction at high n_s to an activated conduction at low n_s in the p- as well as the n-type inversion layers. Since the fixed charge at the interface Q_{ss} in both the p- and n-type inversion layers of our samples is positive, the observed activated conductivity cannot result from carriers bound to the charged interface centers, as these centers are repulsive in the p-type layer. On the other hand, potential fluctuations at the interface can create localized tail states in the sub-band of the p- as well as the n-type layers. This fact in itself strongly suggests that a model based on trapping of the electrons or holes by conventional bound states associated with fixed interface charges is not applicable and favors a more generalized localization by potential fluctuations. Second, at sufficiently low temperatures, the dc resistivity of the inversion layers departs from a simple exponential dependence in a manner consistent with $\exp[(T_0/T)^{1/3}]$ which is expected for Mott's variable-range hopping conduction[4] in a 2D system. Third, weak oscillations (as measured by $\Delta\sigma/\sigma \sim 5\%$) in the magnetoresistance as a function of n_s together with cyclotron-resonance measurements[7] indicate no substantial perturbation of the 2D density of states at energies near the transition to metallic conductivity. In the remainder of this Letter we describe in detail the results for one of the devices.

Figure 1 shows the temperature dependence of the channel resistivity ρ of an n-channel Si MOSFET from 4.2 to 0.4°K [$\rho = (W/l)R$, where w and l are, respectively, the width and the length of the channel and R is its resistance]. This device

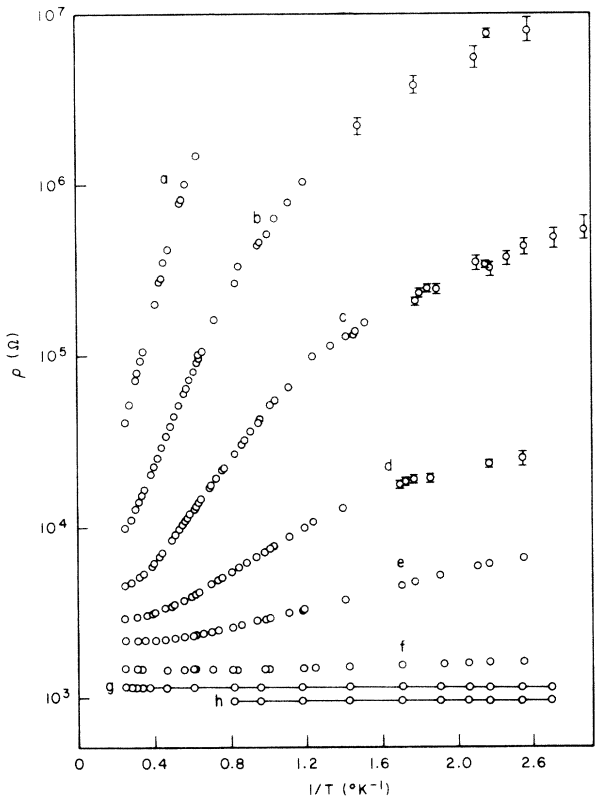

FIG. 1. $\ln\rho$ versus $1/T$ at various surface-carrier concentrations. Curve a, $n_s = 4\times10^{11}/\text{cm}^2$; b, $n_s = 5.2\times10^{11}/\text{cm}^2$; c, $n_s = 6.4\times10^{11}/\text{cm}^2$; d, $n_s = 7.5\times10^{11}/\text{cm}^2$; e, $n_s = 8.7\times10^{11}/\text{cm}^2$; f, $n_s = 1.1\times10^{12}/\text{cm}^2$; g, $n_s = 1.3\times10^{12}/\text{cm}^2$; and h, $n_s = 1.6\times10^{12}/\text{cm}^2$. n_s is determined to $\pm 0.2\times10^{11}/\text{cm}^2$.

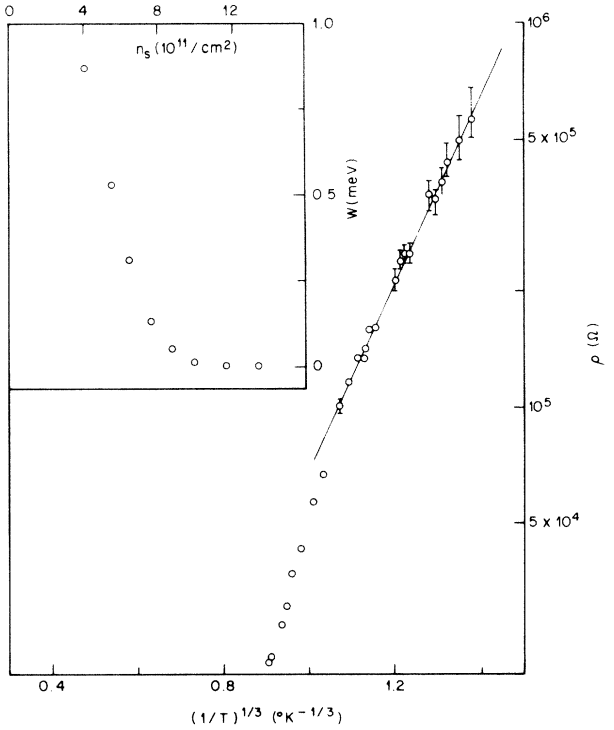

FIG. 2. $\ln\rho$ versus $(1/T)^{1/3}$ at $n_s = 6.4\times10^{11}/\text{cm}^2$. The slope of the solid line gives the parameter $T_0 = 177$°K. The inset shows the activation energy W as a function of n_s.

is fabricated on a (100) surface of a p-type, 10 000-Ω-cm resistivity substrate.[8] The gate oxide, grown by wet oxidation, is 4000 Å thick with $Q_{ss} = 1.2\times10^{11}/\text{cm}^2$ (as determined from C-V measurements). The surface electron density is determined by $n_s = C_0(V_g - V_T)/e$, where C_0 is the oxide capacitance, V_g is the gate voltage, and V_T is the conductance threshold voltage at 78°K. It is well known that n_s determined by using the threshold voltage at 78°K agrees with that obtained from oscillatory magnetoresistivity measurements.[2,9] The temperature is measured by a Ge thermometer accurate to ~1% for $T \gtrsim 0.8$°K and ~3% for $T \lesssim 0.8$°K. Except for the data points with error bars, ρ is accurate to ~2%. We have taken care to avoid carrier heating in the channel.[10]

In this sample, the metallic conduction, which is characterized by ρ being independent of T, is seen at $n_s \gtrsim 1\times10^{12}/\text{cm}^2$. At lower n_s, ρ depends strongly on T. Except for a small temperature range near 4.2°K, the dependence on T for a given n_s can be attributed to an activated conduction described by $\rho \sim e^{W/kT}$ at high temperatures in a reasonably large range of ρ. The activation energy W deduced from these data is shown in the inset of Fig. 2 as a function of n_s. It varies continuously from 0.87 meV at $n_s = (4\pm0.2)\times10^{11}/\text{cm}^2$ to zero at $n_s = (1\pm0.02)\times10^{12}/\text{cm}^2$.

On the basis of these data, we assign a mobility edge separating the localized from the extended states at an energy E_c which equals the Fermi energy E_F at $n_s = 1.0\times10^{12}/\text{cm}^2$. We know from the oscillatory magnetoresistivity measurements that the electron density of states η at this energy does not deviate appreciably from that of the unperturbed 2D sub-band with $\eta = 1.7\times10^{11}/\text{cm}^2$ meV. Further, from the cyclotron-resonance experiments,[10] we exclude the possibility of carrier freezeout in discrete traps. From the density of states and the critical electron density, $\sim 1\times10^{12}/\text{cm}^2$, we determine E_c to be 6 meV above the unperturbed band edge of the 2D sub-band. We note that the activation energy W determined

from our data is substantially less than $E_c - E_F$. For instance, at $n_s = 5.2 \times 10^{11}/\text{cm}^2$, E_F is 3 meV below E_c but W is ~0.5 meV. Unless E_c drops rapidly with E_F, an unlikely possibility,[11] we may conclude that the conduction in this temperature range does not result from activation of localized electrons into the extended states above E_c. We attribute the observed activated behavior to Mott's nearest-neighbor hopping conduction.[4]

The temperature dependence of ρ at still lower temperatures cannot be explained by a temperature-independent activation energy. Deviations from the $e^{W/kT}$ dependence are apparent in Fig. 1 in the data for $n_s = 5.2 \times 10^{11}/\text{cm}^2$ at $T \lesssim 1.2$°K and in the data for $n_s = 6.4 \times 10^{11}/\text{cm}^2$ at $T \lesssim 1$°K. The error bars attached to the data points indicate the uncertainties in determining ρ, which is the channel resistivity in the limit of applying zero voltage across the source and drain. Within the experimental uncertainties, these two sets of data are consistent with an $\exp[(T_0/T)^{1/3}]$ dependence expected for Mott's variable-range hopping conduction in a 2D system. In Fig. 2, the data for $n_s = 6.4 \times 10^{11}/\text{cm}^2$ are replotted on a $\ln\rho$-versus-$(1/T)^{1/3}$ scale. It is clear that ρ follows the $\exp[(T_0/T)^{1/3}]$ dependence on T for $T \lesssim 1$°K. However, the temperature range is much too limited to determine unambiguously the correct power of $1/T$.

The parameter T_0 deduced from our data is 500°K for $n_s = 5.2 \times 10^{11}/\text{cm}^2$ and 180°K for $n_s = 6.4 \times 10^{11}/\text{cm}^2$. According to Mott's argument, $T_0 \approx 27\alpha^2/\pi k\eta$ in the case of a 2D system. Here k is the Boltzmann constant and α^{-1} is the range of the localized state. Our data yield $\alpha^{-1} \approx 110$ Å for $n_s = 5.2 \times 10^{11}/\text{cm}^2$ and ≈ 180 Å for $n_s = 6.4 \times 10^{11}/\text{cm}^2$. We can also estimate α^{-1} from[4] $\alpha(E_F) \approx [2m^*(E_c - E_F)/\hbar^2]^{1/2}$. Using $m^* = 0.2m_0$ and $E_F = n_s/\eta$, we obtain $\alpha^{-1} \approx 80$ Å for $n_s = 5.2 \times 10^{11}/\text{cm}^2$ and $\alpha^{-1} \approx 100$ Å for $n_s = 6.4 \times 10^{11}/\text{cm}^2$.

It is interesting to point out that for both p- and n-type samples the minimum metallic conductivity[12] $\sigma_{\min}$ measured is $\sim 6 \times 10^{-4}\ \Omega^{-1}$, independent of peak mobility, substrate doping, and interface-charge concentration. (Six samples were used, three n channels on 10- and 10 000-Ω-cm p substrates and three p channels on 100- and 10-Ω-cm n substrates, all with $Q_{ss} \geq 0.8 \times 10^{11}/\text{cm}^2$ and $\leq 1.2 \times 10^{11}/\text{cm}^2$.) Although we do not wish to comment on the validity of such a concept, we note that in a 2D system the so-called "minimum metallic conductivity" is relatively insensitive to material parameters, i.e., $\sigma_{\min} \approx k_F\lambda e^2/2h$, where $k_F\lambda$ is the product of the Fermi wave vector and the electron mean free path at the transition. $\sigma_{\min} \approx 6 \times 10^{-4}\ \Omega^{-1}$ gives $k_F\lambda \approx 7$, 7 times larger than the estimate made by Edwards and Thouless.[13]

There are a number of interesting caveats that should be brought forward. It is somewhat surprising that one should see magnetoresistance oscillations and cyclotron resonance[8] at Fermi energies where the electrons are in localized states. This is especially so if one considers that the range of localization α^{-1} is of the order of the cyclotron radius (~100 Å at 100 kG). It is possible that cyclotron resonance survives at low densities because the frequency at which the resonance is observed is sufficiently high. It is, however, not large compared to $E_c - E_F$. Magnetoresistance oscillations in the dc conductivity might exist by virtue of the relative strength of the density of states in 2D in the presence of a magnetic field. Neither explanation is particularly satisfactory. In a sense, we have the rather remarkable result that cyclotron resonance and the magnetoresistance oscillations can be understood in terms of free electrons at densities where nearly all electrons are in localized states. On the theoretical side, we would like to point out that for $n_s < 3 \times 10^{12}/\text{cm}^2$, the Coulomb interaction energy between electrons exceeds the kinetic energy[1] and therefore many-body effects probably play an important role in any quantitative description of this system. In this regard perhaps one should not dismiss contributions from intrinsic localization phenomena such as described by Wigner.[14]

In conclusion, these experiments indicate that the substantial reduction of electron mobility in these systems at low temperatures and low electron densities is due to localization such as proposed by Mott as distinct from trapping by conventional bound states associated with interface charges. A mobility edge where the density of states is only weakly perturbed, thermally activated hopping as distinct from thermal promotion to states above the mobility edge, and variable-range hopping at low temperatures all support such an interpretation. We also note that the minimum metallic conductivity proved quite insensitive to carrier type and to sample characteristics, which may lend some credibility to the concept of a minimum metallic conductivity.

Note added.—After the submission of this manuscript we became aware of similar results by Pepper, Pollitt, Adkins, and Oakley.[15] We thank them for the communication.

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[1]See, for example, J. L. Smith and P. J. Stiles, Phys. Rev. Lett. 29, 102 (1972).

[2]F. F. Fang and A. B. Fowler, Phys. Rev. 169, 619 (1968).

[3]N. F. Mott, Electron. Power 19, 321 (1973).

[4]N. F. Mott and E. A. Davis, *Electronic Processes in Noncrystalline Materials* (Oxford Univ. Press, London, England, 1971).

[5]F. Stern, in "Critical Reviews in Solid State Sciences" (to be published), and unpublished; R. A. Abram, J. Phys. C: Proc. Phys. Soc., London 6, L379 (1973), and references contained therein.

[6]F. Stern and W. E. Howard, Phys. Rev. 163, 816 (1967).

[7]S. J. Allen, Jr., D. C. Tsui, and J. V. Dalton, Phys. Rev. Lett. 32, 107 (1974).

[8]The source and drain are produced by diffusing phosphorus into the substrate to a level of $5\times10^{20}/\mathrm{cm}^3$. The contact resistance is less than 10 Ω in the temperature range of interest here. The resistance is determined by two-terminal measurements, so that one must carefully consider the possibility that the observed behavior may be due to contact effects between the source, drain, and channel. First, we cannot envision significant contact resistance in the properly fabricated MOSFET. Second, we have observed contact effects in some poorly fabricated MOSFETs and find that the contact problem manifests itself at large surface-electron densities where the channel resistance drops substantially below the contact resistance. At low electron densities, high channel resistance, the contact resistance even in these rejected MOSFETs was no problem. Lastly, we note that there are documented in the literature four-terminal measurements at least down to 4.2°K that give the same threshold behavior as seen in two terminal measurements (see Ref. 2).

[9]A. B. Fowler, F. F. Fang, W. E. Howard, and P. J. Stiles, Phys. Rev. Lett. 20, 901 (1966).

[10]F. F. Fang and A. B. Fowler, Phys. Rev. 41, 1825 (1970).

[11]Screening of the potential fluctuations by the free carriers should make E_c increase as n_s decreases. Potential fluctuations from surface roughness, however, might be expected to increase with n_s. The effect of electron-electron interactions on the dependence of E_c on n_s is not clear, but is probably important.

[12]The behavior of σ near E_c at $T=0$ has been a subject of controversy. While Mott proposes that σ is discontinuous at E_c with a minimum metallic conductivity, Cohen, Thouless, and Eggarter suggest that σ tends to zero continuously at E_c: See, for example, N. F. Mott, Phil. Mag. 26, 1015 (1972); M. H. Cohen, J. Non-cryst. Solids 4, 391 (1970), and Phys. Today 24, 26 (1971); D. J. Thouless, J. Non-cryst. Solids 8/10, 461 (1972); T. P. Eggarter, Phys. Rev. A 5, 2496 (1972).

[13]J. T. Edwards and D. J. Thouless, J. Phys. C: Proc. Phys. Soc., London 5, 807 (1972).

[14]E. P. Wigner, Phys. Rev. 46, 1002 (1939), and Trans. Faraday Soc. 34, 678 (1938); A. V. Chaplik, Zh. Eksp. Teor. Fiz. 62, 746 (1972) [Sov. Phys. JETP 35, 395 (1972)].

[15]M. Pepper, S. Pollitt, C. J. Adkins, and R. E. Oakley, Phys. Lett. 47A, 71 (1974).

Theory of Angular Resolved Photoemission from Adsorbates

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A theory of the angular resolved photoemission from localized adsorbate orbitals is presented in which the effects of the final state are discussed in detail. Numerical results show a strong dependence of the energy-resolved angular distribution on the symmetry of the bonding orbitals and on the geometry of the adsorption site.

The recent experimental verification of the angular dependence in photoemission spectra[1] has stimulated considerable interest in this technique. In the case of clean surfaces, it is likely that information about the bulk energy bands and their possible modifications near the surface may be extracted from the angular and energy dependence. The purpose of this Letter is to demonstrate that the angular distribution from localized adatom levels at the surface is dominated by the symmetry of the adsorption site as well as by the symmetry of the bonding orbitals.[2] This indicates the great potential of angular resolved photoemission as a tool complementary to low-energy electron diffraction (LEED) to analyze geometrical structures at surfaces.