RAPID COMMUNICATIONS

PHYSICAL REVIEW B VOLUME 33, NUMBER 2 15 JANUARY 1986

Absence of a Coulomb gap in a two-dimensional impurity band

G. Timp, A. B. Fowler, A. Hartstein
IBM Thomas J. Watson Research Center, Box 218, Yorktown Heights, New York 10598

P. N. Butcher
University of Warwick, Coventry CV47AL, England
(Received 11 October 1985)

The temperature dependence (30 K > T > 400 mK) and magnetic field dependence (H < 50 kG) of hopping conduction have been measured as a function of impurity concentration and surface electric field in a quasi-two-dimensional impurity band formed in the inversion layer of a sodium-doped Si metal-oxide-semiconductor field-effect transistor. We find that our observations can be accommodated by noninteracting, single-particle hopping models based on percolation theory in which the effect of Coulomb interactions between electrons on different sites is ignored. Our observations are not consistent with the existence of a Coulomb gap in the single-particle excitation spectrum, although the gap was expected to determine the conductivity under the conditions examined in these experiments.

Two different models based on classical percolation theory have been proposed to describe hopping conductivity in a two-dimensional (2D) impurity band. Hayden and Butcher[1] have developed a model in which the electrical conductivity is determined by noninteracting particles hopping from singly occupied to vacant sites in a uniform density of localized states, while the Coulomb repulsion between electrons on different sites is ignored. According to this model the conductivity is activated for temperatures $kT > W$ because of a finite bandwidth W in the single-particle excitation spectrum, and follows a $\sigma(T)=\sigma_0(T)e^{-(T_0/T)^{1/3}}$ law at low temperature ($kT << W$). The parameter $T_0=\lambda\alpha^2/\rho$, where α is the exponential decay rate of the localized state, ρ is the density of states, k is the Boltzmann constant, and λ is a constant. In a second model, Efros and Shklovskii,[2] and Pollak[3] have argued that the intersite Coulomb repulsion between electrons cannot be neglected and that the effect of the repulsion is to reduce the number of low-energy one-particle hops about the Fermi level so that the conductivity is determined by excitations across a (Coulomb) gap in the single-particle density of states. For $T > T_c=e^4/\kappa\alpha\rho$ the transport is activated corresponding to excitations across the gap, while at low temperatures $T << T_c$ the conductivity is given by $\sigma=\sigma_0 e^{-(T_0/T)^{1/2}}$, where the temperature $T_0=\lambda' e^2\alpha/\kappa$, κ is the permittivity, and λ' is a constant.

We have measured the temperature dependence (30 K > T > 400 mK) of hopping conduction in a quasi-2D impurity band formed in the inversion layer of a sodium-doped Si metal-oxide-superconductor field-effect transistor (MOSFET) at a series of substrate biases and sodium concentrations, and compared the results with the noninteracting model due to Hayden and Butcher,[1] and the interacting model due to Efros and Shklovskii.[2] We find that our observations can be accommodated by the noninteracting model in which the effect of Coulomb interactions between electrons on different sites is ignored, and we are able to determine the dependences of the parameters of the theory, α and ρ, on substrate bias and impurity concentration. Alternatively, if we fit $\sigma(T)$ with a form which is consistent with the interacting model, we find that the localization length α^{-1} derived from the fit is unrealistically large, and that, under optimum test conditions in which the range of measurable conductivity and accessible temperature are maximized, the functional form of the conductivity exponent predicted by Efros and Shklovskii is not consistent with the measured temperature dependence. In addition, we have measured the magnetic field dependence of the conductivity at fixed temperatures and the temperature dependence of the conductivity in the variable-range-hopping regime for fixed magnetic fields such that $(c\hbar/eH)^{1/2} >> \alpha^{-1}$. We find that the change in the conductivity in a magnetic field at low temperature is described by a law which is consistent with the noninteracting model: $\ln[\sigma(H,T)/\sigma(0,T)] = CH^2/T$, where C is a constant, while Shklovskii[2] predicts a dependence of the form $\ln[\sigma(H,T)/\sigma(0,T)]=CH^2/T^{3/2}$ with a model incorporating a Coulomb gap in the variable-range-hopping regime. Our observations are compelling evidence in support of the noninteracting model and are generally not consistent with the existence of a Coulomb gap in the single-particle excitation spectrum as proposed by Efros and Shklovskii, although the gap should determine the conductivity for the conditions examined in the experiment.

We have made two-point drain-source conductance measurements on three n-channel circular gate MOSFETs as a function of temperature and magnetic field using a lock-in technique at a frequency of 20 Hz. The contact resistance, evaluated by operating the MOSFET above threshold, was observed to be negligible. The conductivity was Ohmic for electric fields less than 1V/cm peak to peak. The MOSFET devices used in these experiments were fabricated on (100) silicon surfaces, and have a channel length of 10 μm and a gate oxide thickness of 100 nm. The gate oxide was purposefully contaminted with NaCl prior to the gate metalization step in the fabrication so that during the experiment the sodium ion concentration near the interface, N_i, could be changed by drifting sodium through the oxide.[4] The ion concentration was determined from the threshold in the transconductance at 77 K.

When the thermal energy is less than the binding energy, electrons in the silicon inversion layer are bound by impurities which are randomly distributed throughout the oxide. When the number of electrons is less than one per site, and the thermal energy is less than the binding energy, the conductivity of the inversion layer is determined by hopping.

The Ohmic hopping conductivity of the inversion layer as a function of gate voltage is shown in the inset of Fig. 1 for a substrate bias of $V_s = 0$ V at $T = 4.21$ K. The maximum in the conductance, which occurs for a gate voltage of 0.95 V corresponding to a carrier density of 4.0×10^{11} cm^{-2}, has been interpreted as evidence of a band in the density of localized states lying (≈ 20 meV) below the lowest electric subband in the silicon.[4] To measure the temperature dependence of the Ohmic conductivity, the gate voltage was adjusted to correspond to the maximum observed in the conductivity at 4.2 K (indicated by the arrow in the figure) which we assume to correspond to a half-filled impurity band. Temperatures as low as 370 mK were obtained using a ^{3}He evaporation cryostat. Figure 1 shows the temperature dependence (400 mK < T < 80 K) of the conductivity observed for a half-filled band under conditions in which the range of sensitivity and temperature accessible in this experiment were maximized. At high temperatures (40 K < T < 80 K) the conductivity is approximately activated corresponding to thermal excitation to the mobility edge. At low temperature (400 mK < T < 30 K) the conductivity is determined by hopping.

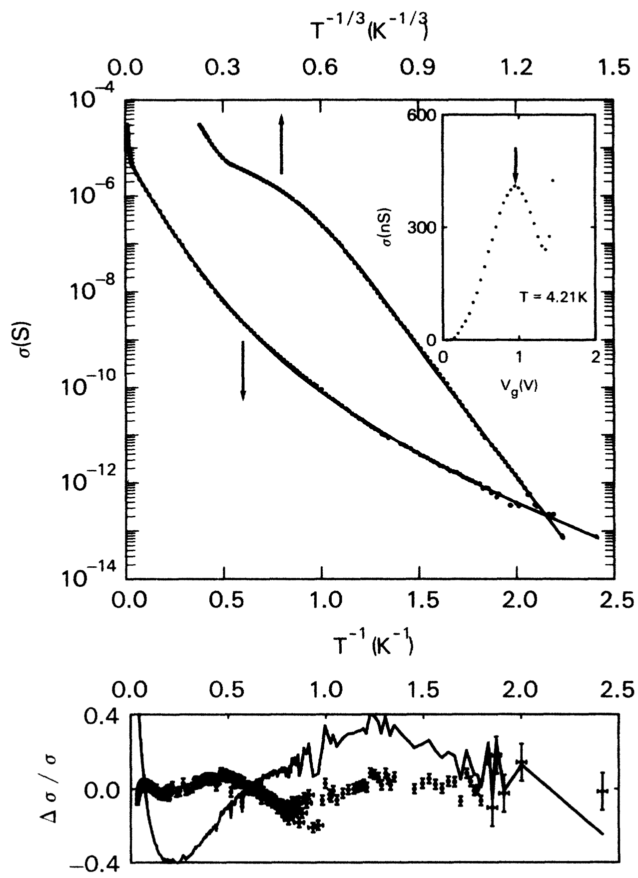

FIG. 1. The temperature dependence of Ohmic conductivity. The solid lines in the figure (which cannot be distinguished from the data points) represent the fit to the data. In the inset, the dependence of the MOSFET channel conductivity on gate voltage below threshold is shown. The lower portion of the figure represents the deviation of the representative data $\Delta\sigma/\sigma = (\sigma_{\text{fit}} - \sigma_{\text{obs}})/\sigma_{\text{obs}}$ from the fit using the HB model (points with error bars) and the interacting model (line).

The observed temperature dependence of a half-filled band is consistent with the model developed by Hayden and Butcher[1] (HB) for hopping conduction in a 2D impurity band in which the density of states $\rho = N_i / W$, and the coefficient of exponential decay of the localized state α are assumed to be constant over a bandwidth W. The structure of the bound-state wave function is taken to be the same as that of an isolated impurity, and the contribution to the site energy arising from the overlap between neighboring sites is assumed to be negligible. According to Hayden and Butcher, the calculation of the dc hopping conductivity in a 2D impurity band of finite width reduces to the problem of calculating the conductivity of an equivalent Miller-Abrahms (MA) conductance network where the conductances represent the transition rates for noninteracting single electron hops between sites. The approximation which is adopted for the Ohmic conductance between two sites (i,j) is

$$G_{ij} = \sigma_0 e^{-2\alpha r_{ij} - \frac{|\epsilon_i| + |\epsilon_j| + |\epsilon_i - \epsilon_j|}{2kT}} = \sigma_0 e^{-\xi_{ij}} , \quad (1)$$

where the intersite distance r_{ij} and the site energies ϵ_i are random variables, σ_0 is a constant, and the site energies are measured relative to the chemical potential. Since the exponent is the conductivity, ξ_{ij} is the sum of random variables, the individual resistances have an exponential scatter. Consequently, the overall electrical conductivity of the network is determined by the critical percolation conductance G_c, defined as the largest value of the conductance such that the subset of resistors with $G_{ij} > G_c$ still contains a connected network which spans the entire system.

The critical percolation conductance is determined by calculating N_c, the number of conductances per site which link the individual sites to the network. N_c is assumed to be invariant at the percolation threshold depending only on the dimensionality and topography of the system. Once the critical conductance is determined, the conductivity of the network is given by a configurational average over all conductances in the neighborhood of G_c. The result of the configurational average is

$$\sigma = g_0 \sigma_c e^{-\xi_c} . \quad (2)$$

The prefactor σ_c in Eq. (2) represents the contribution to the conductivity of the other resistors ($G_{ij} \neq G_c$) in the MA network. The prefactor g_0 is proportional to the hopping rate and is assumed to be a constant independent of temperature in our analysis. Analytical expressions for ξ_c and σ_c used in the analysis of the data are derived explicitly in Ref. 1. We note that for $\xi_c < W/2kT$ the Ohmic conductivity has the form $\sigma(T) \sim (T/T_0) e^{-(T_0/T)^{1/3}}$, where $kT_0 = 13.75\alpha^2/\rho$ corresponding to the variable-range-hopping law in 2D, while for $W/kT \leq \xi_c$ the transport is approximately activated, with an activation energy corresponding to $5W/12$.

To estimate the localization parameter α, the bandwidth W, and the prefactor g_0, the data as a function of temperature are fit to the HB model over the applicable temperature range which is determined self-consistently for a given choice of parameters. The data are fit by solving for ξ_c and σ_c at each temperature for an initial estimate of the parameters α, W, and g_0, and then substituting the results into Eq. (2). The choice of parameters is subsequently refined using a nonlinear fitting algorithm to minimize the least-squares deviation of the fit from the data. A typical fit is represented in Fig. 1 by the solid line. In the figure, the same conductivity data are plotted against both $T^{-1/3}$ and T^{-1} to emphasize the temperature regimes in which the conditions $\xi_c < W/2k_BT$ and $W/k_BT < \xi_c$ apply. For the data shown, the entire range where the model applies (i.e., from $\xi_c < W/2k_BT$ to $W/k_BT < \xi_c$) must be used to fit the data. The lower portion of Fig. 1 represents the relative deviation of the fit from the data $\Delta\sigma = (\sigma_{\rm fit} - \sigma_{\rm obs})/\sigma_{\rm obs}$. The theory is consistent with the temperature dependence of the Ohmic conductivity observed over seven orders of magnitude variation in the conductivity in the temperature range 30 K $> T >$ 400 mK within the experimental error.

The values of the parameters α, W, and g_0 deduced from the fit to the data are of the order expected. The parameter α^{-1} which has a value of 3.17 nm for the data of Fig. 1 is approximately the localization length 2.10 nm of the ground-state wave function corresponding to a 2D Coulombic impurity potential. The bandwidth, which has a value of 3.75 meV, is less than the Coulomb scatter of the energy levels, $e^2N_i^{1/2}/\kappa \sim 13$ meV, where $\kappa = 7.7$ is the average permittivity at the interface. The parameter $g_0 = 53.3$ mS is sensitive to minute changes in W and α. If we assume on the basis of a dimensional argument that $g_0 \simeq e^2R_0/k_BT$ and determine a value for the characteristic hopping rate R_0, we find that $R_0 \simeq 10^{13}$ sec^{-1} at 4 K which is the correct order of magnitude.

By changing the sodium concentration, and the surface electric field using a substrate bias, the HB model can be evaluated for a variety of different values of the parameters α, W, and g_0. For example, if we change the sodium concentration at constant substrate bias and filling fraction, then the parameter α should not change since the structure of the wave function is, by hypothesis, the same as for an isolated impurity independent of the sodium concentration, but the density of states changes because $\rho = N_i/W$. However, if we apply a negative substrate bias at a fixed sodium concentration and filling fraction, the exponential decay rate of the wave function increases because the binding energy increases.[4]

The inset of Fig. 2 summarizes the dependence of α^{-1} on sodium concentration and substrate bias observed for a half-filled band in one sample. We find that α is relatively independent of sodium concentration and increases with increasing substrate bias in correspondence with our expectations. The trends observed in the bandwidth as a function of the overlap between sites measured by the product $\alpha N_i^{-1/2}$, where $N_i^{-1/2}$ is the intersite distance, are shown in Fig. 2. The overlap was varied by changing both concentration and surface field. We observe that the bandwidth increases as the overlap between neighboring impurity sites decreases. For a constant substrate bias, we find that the density of states decreases as the sodium concentration decreases which is expected since $\rho = N_i/W$, but that the bandwidth W must increase as the sodium concentration decreases to accommodate the data. At a fixed concentration, we observe that the density of states decreases as the substrate bias decreases because the bandwidth increases. The trend observed in W is not understood, but the data are consistent with the assumption that the overlap energy[2] $\Delta\epsilon = E_b \exp(-\alpha N_i^{-1/2})$ is negligible which is implicit in the HB model. For a binding energy of $E_b = 20$ meV, $\Delta\epsilon = 0.1$ meV $<< W$.

We have shown that the observed temperature dependence of Ohmic hopping conduction in a 2D impurity band is consistent with the HB model. The effect of the intersite Coulomb interaction $E_c \sim e^2N_i^{1/2}/\kappa$ is ignored in the model used to analyze the data, but the gap which results in the single-particle excitation spectrum as a result of the Coulomb repulsion is estimated[3] to be $\Delta \sim E_c\sqrt{E_c/W} \sim 10$ meV. It should not be legitimate to ignore the Coulomb repulsion if it is comparable to the disorder energy W or the thermal energy. The depletion of the low-energy excitations

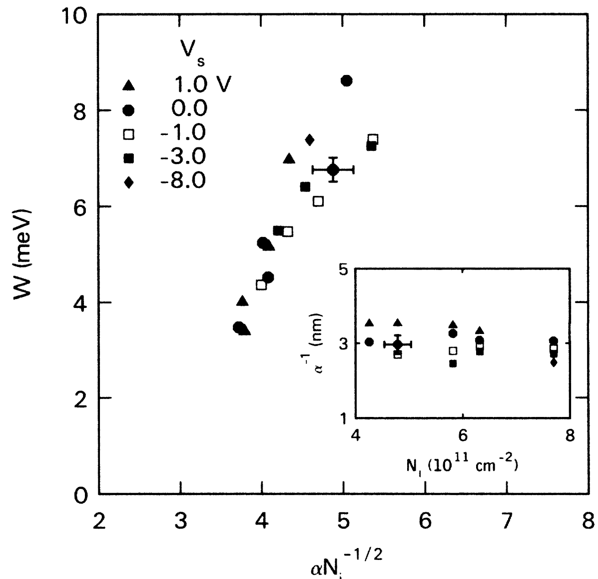

FIG. 2. The bandwidth W deduced from the temperature dependence as a function of the overlap $\alpha N_i^{-1/2}$. In the inset, the dependence of α^{-1} on substrate bias and sodium concentration is shown.

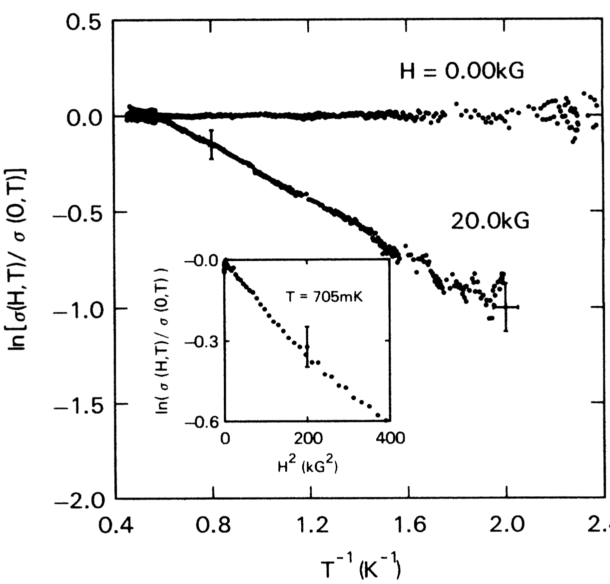

FIG. 3. The temperature dependence of the relative change in the conductivity in magnetic fields of 0.00 and 20.0 kG, respectively. The 0.00 kG is the ratio of two separate experimental results and exemplifies the reproducibility. The inset shows the quadratic magnetic field dependence of the conductivity in the variable-range-hopping regime.

by the Coulomb interaction impedes variable-range hopping for temperatures $T < T_c = e^4 N_i / \kappa \alpha W$ and results in activated conductivity. At low temperature the conductivity is given by $\sigma \sim \exp[-(T_0/T)^{1/2}]$, where the temperature $kT_0 = 6.2 e^2 \alpha/\kappa$.

If we fit the low-temperature conductivity data for a half-filled band to this functional dependence over a temperature range in which the optimum exponent is one half (400 mK $< T <$ 20 K in Fig. 1), we find that the conductivity consistently deviates from a $T^{-1/2}$ dependence (see the line in the lower portion of Fig. 1), and that the localization length α^{-1} deduced from T_0 assuming $\kappa = 7.7$ varies between 22.1 and 42.3 nm depending on the substrate bias and sodium concentration. This estimate of the localization length is one order of magnitude larger than the length of the wave function associated with the Coulombic potential of the impurity near the interface. The exponential decay rate necessary to fit the data is unrealistic so that the conductivity observed at low temperature is larger than that predicted by the interacting model.

In a further attempt to unambiguously determine the temperature dependence of the exponent in the conductivity in the variable-range-hopping regime, we measured the temperature dependence of a half-filled band in a magnetic field. A weak magnetic field changes the conductivity exponent ξ_{ij}, viz., $\Delta \xi_{ij} = r_{ij}^3 / 12 \lambda^4 \alpha$. Since the characteristic hopping length is practically unaffected by a magnetic field, the principal contribution to ξ_c is given by $\xi_c^3/(\alpha\lambda)^4$, so that the low-field magnetoresistance should be positive and have the form

$$\ln\left[\frac{\sigma(H,T)}{\sigma(0,T)}\right] = \frac{Ce^2H^2}{c^2\alpha^4\hbar^2}\xi_c^3 \ , \tag{3}$$

where C is a negative constant. In the noninteracting model $\xi_c = (T_0/t)^{1/3}$ so that $\ln[\sigma(H,T)/\sigma(0,T)] \sim H^2/T$, while in the interacting model $\xi_c = (T_0/T)^{1/2}$ so that $\ln[\sigma(H,T)/\sigma(O,T)] \sim H^2/T^{3/2}$. Figure 3 shows the temperature dependence of the magnetoconductivity of a half-filled band in the temperature regime in which the zero-field conductivity is determined by variable-range hopping and in the magnetic field regime in which the exponent of the magnetoconductivity is proportional to H^2. To obtain the curves shown in the figure, the logarithm of the zero-field conductance was subtracted from the temperature dependence of the logarithm of the magnetoconductance at 0.00 and 20.0 kG, respectively. We observe that the temperature dependence of the magnetoconductivity is consistent with the T^{-1} dependence predicted by the noninteracting model.

[1]K. J. Hayden and P. N. Butcher, Philos. Mag. B **38**, 603 (1979).

[2]A. L. Efros and B. I. Shklovskii, J. Phys. C. **8**, L49 (1975); B. I. Shklovskii and A. L. Efros, in *Electronic Properties of Doped Semiconductors*, edited by M. Cardona, P. Fulde, and H. T. Queisser, Springer Series in Solid-State Sciences, Vol. 45 (Springer-Verlag, Berlin, 1984).

[3]M. Pollak, Discuss. Faraday Soc. **50**, 13 (1970).

[4]T. Ando, F. Stern, and A. B. Fowler, Rev. Mod. Phys. **54**, 437 (1982); A. B. Fowler and A. Hartstein, Philos. Mag. B **42**, 949 (1980).