sume the value of E_{sp} reported in Ref. 4, we are able, on the basis of our data of Fig. 1, to draw the exact configuration of the RES structure including the shape and the location of the potential wells in the configurational space. We shall consider thoroughly these important details in a following, more extended paper.

Observation of Higher Sub-band in *n*-Type (100) Si Inversion Layers

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We have observed population of the heavy-mass sub-band in *n*-type (100) Si inversion layers at an electron density of $(7.4 \pm 0.3) \times 10^{12}/\mathrm{cm}^2$, corresponding to an energy splitting of 46 meV. These data are inconsistent with results from recent self-consistent-field calculations and confirm that the many-body effects are important.

The *n*-type inversion layer on a (100) surface of *p*-type Si has been the subject of many recent studies.[1-7] Although its relatively high electron mobility has led to extensive studies of the electronic properties, especially by using the Shubnikov–de Haas (SdH) effect[1,2] and the cyclotron resonance,[4,5] the energy of its first few quantum levels is still uncertain. Fang and Howard[8] first pointed out that the six conduction ellipsoids are not equivalent in this surface inversion layer. The ground-state energy level, E_0, associated with the two ellipsoids whose long axes are perpendicular to the surface, is lower in energy than E_0', the ground-state energy level associated with the other four ellipsoids. The cyclotron mass characterizing the electronic motion parallel to the surface is $m^* = 0.190 m_0$ for sub-bands of the two lower-energy ellipsoids and $m^* = 0.417 m_0$ for sub-bands of the higher-energy ellipsoids. According to their variational calculations, population of the heavy-mass sub-band of E_0' should begin when the electron density (n_s) in the inversion layer exceeds $(3-5) \times 10^{12}/\mathrm{cm}^2$. Subsequent self-consistent-field calculations by Stern[6] and by Pals[7] predict that E_0' and E_1 (the first excited-state level of the two lower ellipsoids) are close in energy. At $T = 0$ K, E_1 lies below E_0' and population of the E_1 sub-band should begin at $n_s \approx 3 \times 10^{12}/\mathrm{cm}^2$. As SdH and cyclotron-resonance experiments, carried out in this n_s range, have failed to detect the population of any higher sub-bands,[2,5] it becomes suggestive that many-body effects are important in determining these energy level splittings. More recent calculations[9-12] of the exchange and correlation energy of electrons in the E_0 sub-band and its effects on the electron mass and the g factor tend to support this thesis.

In an effort to study quantum effects in Si inversion layers under compressional stresses, we have studied the SdH effect in *n*-type (100) Si inversion layers at high electron densities (up to $3 \times 10^{13}/\mathrm{cm}^2$) and have observed the population of a higher sub-band at a threshold electron density $n_{st} = 7.4 \times 10^{12}/\mathrm{cm}^2$. The fact that n_{st} decreases when a compressional stress is applied is evidence that this higher sub-band is the heavy-mass sub-band associated with E_0'. In the rest of this Letter, we shall present these results and discuss their implications for the energy structure and the many-body effects in the inversion layer. Population of higher sub-bands in Si inversion layers on (322), (211), (311), and (811) surfaces has already been reported by Lakhani and Stiles.[13] Kamgar *et al.*[14] have observed optical transitions between the two lowest sub-bands in the accumulation layer on *n*-type (100) Si. Wheeler and Ralston[15] have reported optical transitions from E_0 to E_2 and several higher sub-bands in photoconductivity measurements.

Our experiments were performed on circular metal-oxide-semiconductor field-effect transistors fabricated on the (100) surface of 25-Ω-cm *p*-type Si. The gate oxide is thermally grown to 1080 Å thick. The maximum electron mobility of these samples at 4.2 K is ~6000 cm^2/V sec. The SdH effect was studied at 4.2 K, with use of a superconducting magnet capable of fields up to 70 kG. We found that in order to resolve the SdH oscillations at large gate voltage (V_g), where the electron mobility is extremely low, it was necessary to measure the second derivative of the curve of drain current (I_d) versus V_g, i.e., d^2I_d/dV_g^2, by using standard modulation techniques.[16] In this case, we modulate the gate voltage at 500 Hz and measure d^2I/dV_g^2 by detecting the ac com-

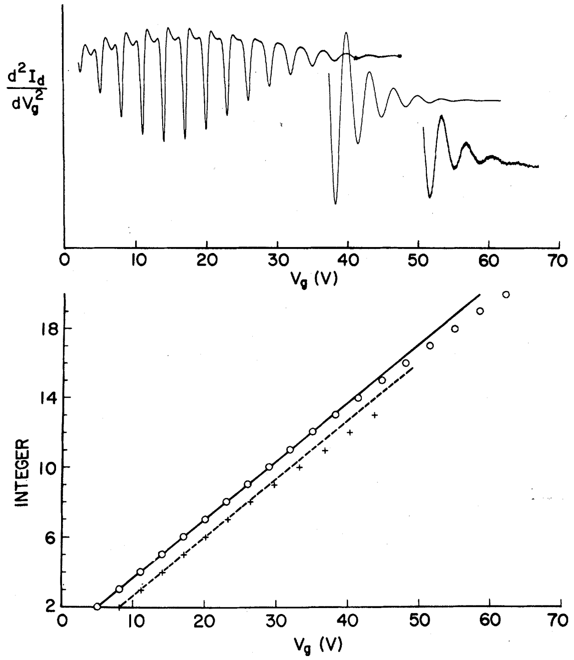

FIG. 1. The Shubnikov–de Haas oscillations in d^2I_d/dV_g^2 versus V_g from an n-type (100) Si inversion layer (sample np5701) at 4.2 K with $H=60$ kG applied perpendicular to the plane of the Si-SiO$_2$ interface. A change in scale by a factor of 25 was used for the trace starting at $V_g \sim 37$ V and by 20 for that starting at ~ 50 V. The lower panel shows N versus V_g. The circles are from the d^2I_d/dV_g^2-versus-V_g curve shown in the upper panel and the crosses are taken from the same sample when a uniaxial compressional stress is applied along a ⟨110⟩ direction in the plane of the interface.

ponent of the drain current at 1000 Hz with a phase-sensitive detector.

The upper panel of Fig. 1 shows the SdH oscillations in a d^2I_d/dV_g^2-versus-V_g plot at a magnetic field $H=60$ kG, applied perpendicular to the plane of the Si-SiO$_2$ interface. The oscillation amplitude shows strong dependence on V_g. It reaches a maximum at $V_g \sim 15$ V and decreases to approximately one percent of its maximum value at $V_g \approx 50$ V. This strong dependence on V_g is a reflection of the V_g dependence of the electron mobility in the inversion layer.[17]

The period of these oscillations is the change in V_g which produces a change in n_s equal to the number of electrons needed to fill a Landau level. This number is $4eH/hc$ (here, e is the electronic charge, c is the velocity of light, and h is Planck's constant) for electrons in the E_0 subband. Consequently, the dips in the d^2I_d-versus-V_g curve occur whenever V_g satisfies

$$V_g = N(4e^2/C_0hc)H + V_0, \tag{1}$$

where V_0 is a constant, C_0 is the oxide capacitance, and N is an integer. Thus, if we label the dips in the d^2I_d/dV_g^2-versus-V_g curve from left to right by integers $N=1, 2, 3\ldots$, a plot of N against V_g at which the dips occur should yield a straight line. The circles in the lower panel of Fig. 1 are results from such a plot for the d^2I_d/dV_g^2-versus-V_g curve shown in the upper panel. It is clear that, for $V_g \leq 35$ V, the data points lie on a straight line and N follows a strictly linear dependence on V_g. The rate of change of n_s with respect to V_g, i.e., $dn_s/dV_g = C_0/e$, obtained from the slope of the straight line is $1.94 \times 10^{11}/\text{cm}^2$ V, in good agreement with that calculated from the oxide thickness. Thus, for $V_g \lesssim 35$ V, all the inversion-layer electrons occupy the E_0 sub-band and all the higher sub-bands are empty.

For larger V_g, the data points deviate from the straight line. This deviation is due to population of a higher sub-band.[13] If we draw a straight line through the last five points, we obtain from the slope of this line $dn_s/dV_g = 1.63 \times 10^{11}/\text{cm}^2$ V. The difference between this value of dn_s/dV_g and that obtained from the data at $V_g \lesssim 35$ V gives us the rate of population of the higher sub-band, which is $0.31 \times 10^{11}/\text{cm}^2$ V. This small rate indicates that, as n_s increases further, the Fermi energy increases only slightly faster than the splitting between the bottom of this sub-band and E_0. In other words, the Fermi energy in this higher sub-band increases very slowly. With this rate of filling, the SdH oscillations at 60 kG should have a period of 18 V for the E_1 sub-band and 36 V for the E_0' sub-band. We have attempted and failed to find any hint of long-period oscillations up to $V_g = 100$ V. Our failure strongly suggests that this higher sub-band is not the E_1 light-mass sub-band, but the E_0' heavy-mass sub-band.

That this higher sub-band is the E_0' heavy-mass sub-band becomes evident when a compressional stress is applied along a ⟨110⟩ direction in the plane of the Si-SiO$_2$ interface. Under such a stress, the E_0' sub-band is expected to decrease its energy while the E_0 and E_1 sub-bands are expected to increase their energies.[3,18] Since the SdH oscillations are measured as a function of V_g, we expect the threshold V_g, at which population of the E_0' sub-band begins, to decrease under the stress. On the other hand, no change in the threshold V_g is expected if the higher sub-band being populated is the E_1 sub-band. At smaller V_g, where all the higher sub-bands remain empty under the applied stress, we expect no change in the period of the SdH oscillations and only the d^2I_d/dV_g^2 dips to shift to higher V_g.

The crosses in Fig. 1 show the N-versus-V_g data taken from the same sample when a uniaxial compressional stress of approximately 2×10^9 dyn/cm^2 was applied along a crystallographic $\langle 110\rangle$ direction in the plane of the Si-SiO$_2$ interface. (These data points are displaced downward from the circles by one integer for the sake of clarity.) For $V_g \lesssim 25$ V, the data points lie on a straight line which is parallel to that through the data points at $V_g < 35$ V taken with no applied stress. Thus, no change in the period of the SdH oscillations is observed and only the d^2I_d/dV_g^2 dips are shifted to larger V_g by about 0.2 V. For large V_g, the data points deviate from this straight line and follow the same trend seen in the data points taken with no applied stress at $V_g \gtrsim 35$ V. The fact that this threshold V_g is shifted from ~37 V to ~25 V by the applied stress is a strong evidence supporting our identifying this higher sub-band as the heavy-mass sub-band of E_0'. It should be noted that this shift corresponds to a change in the energy separation between E_0' and E_0 by $\Delta E \sim 14$ meV, which is considerably larger than $\Delta E \sim 9$ meV estimated from the shear deformation potential[18] and the elastic stiffness constants[19] of bulk intrinsic Si. It should also be noted that, under the applied stress, the amplitude of the SdH oscillations was so reduced that we were unable to resolve oscillations at $V_g > 50$ V. Currently, we are preparing for more accurate determination of the stress dependence of this threshold V_g and the amplitude of the SdH oscillations.

We have so far succeeded in measuring the SdH effect at sufficiently high electron densities to allow the observation of this heavy-mass sub-band in four samples and obtained from them consistent results. We deduce from these measurements that the threshold electron density, at which the Fermi level crosses the bottom of the E_0' sub-band, is $n_{st} = (7.4\pm0.3)\times10^{12}/\text{cm}^2$. The energy splitting at this electron density, calculated by using $m^* = 0.19m_0$ for the E_0 sub-band, is $E_0' - E_0 = 46\pm2$ meV. This estimate of the energy splitting between E_0' and E_0 is made without taking into account band tailing in the E_0' sub-band, which is probably unimportant here. We also note that the Si-SiO$_2$ interface resulting from thermal oxidation of Si is known to be in a state of compression.[20,21] The maximum stress in Si has been reported to be $\lesssim 1\times10^8$ dyn/cm^2. In view of our stress experiment discussed earlier, correction for this residual stress may increase $E_0' - E_0$ by $\lesssim 1$ meV, which is also unimportant here.

Our experimental results disagree with predictions from the self-consistent Hartree calculations of Stern[6] and of Pals.[7] Take, for instance, the numerical results of Stern for the (100) inversion layer on p-type Si with an acceptor density of $10^{14}/\text{cm}^3$ (the acceptor density in our samples is $\sim 6\times10^{14}/\text{cm}^3$). His calculations predict that E_1 lies below E_0' in energy and population of the first higher sub-band should begin at $n_s \approx 3\times10^{12}/\text{cm}^2$. Stern[10] first demonstrated the importance of the many-body effects in determining the energy levels of this inversion layer. He found that the exchange energy lowers the E_0 sub-band by an amount comparable to the sub-band splittings resulting from self-consistent Hartree calculations. More recent calculations[11,12] of the many-body effects on the electron mass and its g factor showed qualitative agreement between theory and experiments. Vinter[12] also demonstrated that the correlation energy for electrons in the E_0 sub-band is also comparable to the exchange energy. The fact that our data are inconsistent with results from the self-consistent Hartree calculations gives further evidence that the many-body effects are important in determining the energy structure of this quasi two-dimensional electronic system. We hope that our results can provide some means for testing the various approximate methods for calculating the many-body Coulomb interactions.

In summary, we have observed the population of a higher sub-band in the n-type (100) Si inversion layer and presented evidence showing that this higher sub-band is the heavy-mass ground-state sub-band associated with the four conduction ellipsoids whose long axes lie in the plane of the Si-SiO$_2$ interface. The Fermi energy crosses the bottom of this sub-band when the inversion-layer electron density equals $(7.4\pm0.3)\times10^{12}/\text{cm}^2$, which corresponds to an energy splitting of 46 ± 2 meV between the bottom of this heavy-mass sub-band and the bottom of the light-mass ground-state sub-band. These data are inconsistent with results from the self-consistent Hartree calculations of Stern[6] and Pals[7] and confirm recent suggestions that the many-body effects are important in determining the energy structure of Si inversion layers.

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Metal-Induced Surface States during Schottky-Barrier Formation on Si, Ge, and GaAs

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We report evidence for extrinsic metal-induced surface states during the early stages of Schottky-barrier formation on Si(111), GaAs($\overline{111}$), Ge(111), and Ge(100). Results on Ge(110) are related to those of Eastman and Freeouf for GaAs(110) and GaSb(110) and we propose a simple structural model to account for the anomalous results on (110) semiconductor surfaces.

Although the existence of surface states at the metal-semiconductor interface was proposed by Bardeen[1] in 1947 there has been little direct information about their spectroscopy and chemical origin until recently.[2,3] Eastman and Freeouf[3] have observed intrinsic-surface-state spectra on III-V semiconductors such as GaAs that *persist in the presence of a metal overlayer.* These authors were able to correlate the Schottky-barrier energies[4-6] with intrinsic-surface-state positions and suggested that the barrier height of III-V semiconductors is determined by *intrinsic surface states.* Our results in this paper show that this is *not true* for the (111) surfaces of Si, Ge, and GaAs. Intrinsic surface states on these surfaces are *removed* by the metallic overlayer and new states appear near the Fermi energy which are localized about the metal adatoms. These *extrinsic surface atoms* pin the Fermi energy on (111) and (100) surfaces and determine the Schottky-barrier height. From ultraviolet-photoemission-spectroscopy measurements of bulk band-structure transitions of Si, Ge, and GaAs we deduce band-bending changes with final barriers, $\varphi_B = E_c - E_F$, of 0.75, 0.60, and 0.85 eV, respectively, in good agreement with Schottky-barrier heights measured by conventional capacitance-voltage measurements.[4-6,7] Similar metal-induced surface states occur within the band-gap energy range on Ge(100) surfaces but are much weaker on Ge(110) surfaces. The Ge(110) surface states occur at higher energies than on Ge(100) and Ge(111) and are not *completely* removed by metallic overlayers. A simple structural model is proposed for (110) surfaces in which only one-half of the "normal" surface at-