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Valley-Valley Splitting in Inversion Layers on a High-Index Surface of Silicon

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The superlattice phenomenon observed by Cole, Lakhani, and Stiles in the electron inversion layer on (119)Si is explained by projecting the bulk band structure onto the surface. On high-index surfaces, the valley degeneracy only occurs at the surface-band-structure zone boundary. Lifting this degeneracy gives rise to minigaps which we observe in the optical conductivity as interband absorption.

In a silicon MOSFET (metal-oxide-semiconductor field-effect transistor) with an interface of Si tilted away from the high-symmetry plane (001) to a high-index plane such as (119), Cole, Lakhani, and Stiles[1] have found structures in the dc conductivity and unusual oscillations in the magnetoconductivity. They explained the observed phenomena in terms of a model of a one-dimensional superlattice along the interface. The precise cause of the formation of the superlattice is, however, unknown.

We present an alternative explanation in terms of valley splitting[2,3] between the two conduction-band minima in the [001] direction. The formation of an energy gap in the $[\bar{n}n2]$ direction on the tilted (11n) Si-SiO_2 interface follows naturally and the so-called "superlattice period" as a function of tilted angle is easily explained. Furthermore, we have measured the optical conductivity and observed a peak due to the interband transitions across the minigap. While the dependence of the energy gap on electron density is consistent with both our valley-splitting model and the superlattice model, the observed intensity of the inter-

band peak is better explained by our model.

In n-type Si, there are two conduction-band valleys along [001] at $\pm k_0 = \pm 0.85(2\pi/a)$ where a is the lattice constant, 5.43 Å. In Fig. 1, the surface electron energy vs $\vec{k}$ in the direction $[\bar{n}\bar{n}2]$ on the tilted surface $(11n)$ is plotted. Where the parabolas cross, the valley splitting will cause the formation of a minigap as in the superlattice model. The closest pair of parabolas are separated by $G = 0.3(2\pi/a)\sin\theta$. This vector $\vec{G}$ on the interface determines the density at which the Fermi energy enters the minigap and at which the anomaly in the dc conductivity occurs. L, the period in the superlattice model, is related to G in our model by $L = 2\pi/G$. In Table I, the calculated values are compared with the measured values. Agreement is satisfactory. The large-angle planes, such as (113), were not found to have such structures[1] because the large G value means that the electron density required to fill to the minigap is outside the experimental range. For the same reason, the gap formed between two parabolas at $2k_0\sin\theta$ apart cannot be seen, unless θ is sufficiently small.

According to our theory, the valence band is single valleyed and, therefore, no such valley-splitting structure exists for the p channel on a tilted surface, in agreement with the findings of Cole, Lakhani, and Stiles.[1]

Since there is wave-function mixing concomitant with the gap formation in the coordinate along $\vec{G}$, the projection of the intervalley wave vector through the X point on the interface, there is optical absorption due to electronic transitions across the gap if the oscillating electric field is polarized along $\vec{G}$. The transition matrix element vanishes as $G \to 0$, so that transitions will not be seen on an (001) surface. There is no interband absorption for the polarization perpendicular to $\vec{G}$. This is true no matter what the plane of tilt from (001) is in relation to the crystal axes.

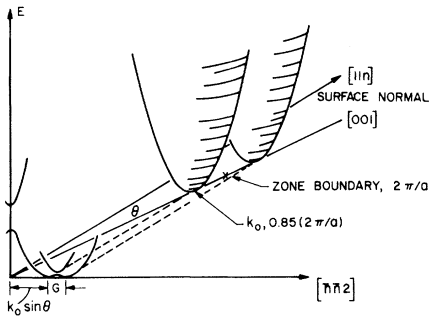

FIG. 1. Curves of energy vs wave vector. If one projects the bulk energy-momentum relation from the two minima along the [001] direction onto the $(11n)$ surface, two parabolas are obtained, spaced by a surface wave vector $\vec{G}$. The valley-valley splitting causes a gap at the crossing.

We measured the real optical conductivity, $\mathrm{Re}\sigma(\omega)$, of the inversion layer for a MOSFET in which the interface normal lies in the (110) plane, 9° from the [001] direction. The peak mobility of the device was $\approx 10\,000$ cm²/V sec. The fixed oxide charge, determined from the 77°K threshold shift, was $Q_{ss} \approx -1.5\times 10^{10}$ cm². The substrate doping was $N_A - N_D \approx 6.5\times 10^{14}/\mathrm{cm}^3$. A thin Ti gate to allow far-infrared radiation to penetrate the device was insulated from the substrate by a 1400-Å oxide.

The real conductivity is directly related to the fractional change in transmission of far-infrared radiation by[4]

$$\Delta T/T \approx 2\,\mathrm{Re}\sigma(\omega)/(Y_O + Y_S + Y_G), \qquad (1)$$

where Y_O, Y_S, and Y_G are the wave admittances of free space, silicon, and the gate metallization, respectively. In this experiment, $\Delta T/T$ is measured with a conventional Fourier transform spectrometer from 5 to 60 cm^{-1}. A polarizer was placed in the path of the radiation so that the optical conductivity could be measured either parallel to $\vec{G}$, $\sigma_{\parallel}(\omega)$, or perpendicular to it, $\sigma_{\perp}(\omega)$. The dc conductivity was measured perpendicular to $\vec{G}$, and the structure reported by Cole, Lakhani, and Stiles[1] was reproduced (curve A, Fig. 1 of Ref. 1). The maximum in $\sigma_{\perp}(0)$, obtained when the Fermi energy and the minigap coincide, occurred at $n_s = 2.5\times 10^{12}/\mathrm{cm}^2$. (This implies that L, in the superlattice model, is ≈ 110 Å, or G in our model is $2\pi/110\ \text{Å}^{-1}$.) All the measurements reported here were taken at 1.2°K.

In Fig. 2 we show both $\sigma_{\parallel}(\omega)$ and $\sigma_{\perp}(\omega)$ as a

TABLE I. Superlattice period ($L = 2\pi/G$).

Sample	Surface	θ	Measured period (Å)	Calculated period (Å)
a	(115)	16°	59–72	66.5
b	(118)	10°	104	104.0
c	(118.9)	9°	110–120	115.7

[a] F. F. Fang and A. B. Fowler, as quoted in Ref. 1.
[b] Cole, LaKhani, and Stiles, Ref. 1.
[c] Our samples.

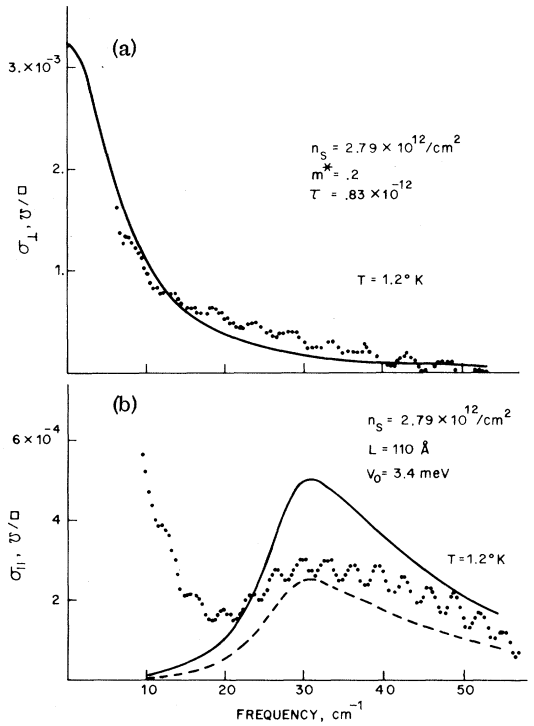

FIG. 2. Optical conductivity vs frequency. (a) $\vec{E}$(infrared) $\perp \vec{G}$; ●, experiment; ——, Drude term. (b) $\vec{E}$(infrared) $\parallel \vec{G}$; ●, experiment; ——, interband contribution from the superlattice model; ---, interband transitions from our valley-splitting model.

function of frequency. (The oscillatory structure is due to interference in the substrate and may be ignored.) For $\sigma_\perp$ we expect Drude-like behavior. Indeed the solid line in Fig. 2(a) is the Drude prediction based on the measured dc conductivity, $\sigma_\perp(0)$, assuming a mass of $0.2m_0$. Although the overall agreement is satisfactory, significant departures may be seen that lie outside both the superlattice model and the valley projection model described here. This is not understood at present. $\sigma_\parallel(\omega)$ exhibits a peak whose position and strength depend on gate voltage. We attribute this peak to interband absorption across the minigap.

The solid curve in Fig. 2(b) is the interband contribution to the conductivity, calculated in the superlattice model with a periodic potential $V = V_0\cos(2\pi x/L)$, for the parameters indicated.[5] Level broadening is included by convoluting it with a Lorentzian whose width is given by the transport τ derived from $\sigma_\perp(0)$ [Fig. 2(a)]. We observe that when the Drude tail is added onto this interband peak, it is much too large compared with the measured conductivity. On the other hand, in our valley-splitting model, because of the removal of the valley degeneracy, the interband contribution, as shown by the dashed curve in Fig. 2(b), is half as big as that in the superlattice model. Adding on the Drude tail would give good agreement with experiment. This is clear evidence in favor of the valley-splitting model. We emphasize that the calculated intensity of interband transitions in both models depends only on the input parameters V_0, L, and τ. Indeed, to fit the data, we adjust only V_0. L is determined from the position of the anomaly in the dc conductivity, and τ from the dc conductivity itself.

At each value of n_s we fitted the interband absorption by adjusting V_0 and extracted the minigap as a function of n_s. The data are shown in Fig. 3 along with some estimates of Cole, Lakhani, and Stiles.[1] Only when the Fermi energy is above the gap can we extract a value for the gap.

Sham and Nakayama[2] have given a theory of the valley splitting. On the n-type Si(001) surface, near the conduction-band minimum, a state with wave vector $k_0 - k$ near the $(0, 0, k_0)$ minimum propagating towards the surface is reflected mainly into a component with wave vector $k_0 + k$ (in the same valley) and with a small probability amplitude ($= \alpha k$, where α is a constant) into another component with wave vector $-k_0 + k$. This coupling of two valleys gives a perturbation $\alpha \partial V/\partial z$, where V is the effective potential, causing valley splitting. For a tilted surface, α depends on the angle of tilt, θ. The energy gap formed at the intersection of the two parabolas in Fig. 1 is, therefore, approximately proportional to the gate voltage and is roughly estimated to be

$$V_0 \sim (0.7\ \text{meV})(1 + 1.4\sin^2\theta)(\gamma n_s + n_d), \qquad (2)$$

where n_s and n_d are, respectively, the surface density of the inversion layer and that of the depletion charges in units of 10^{12} cm^{-2}, and γ is a constant[2] with a value between $\frac{11}{32}$ and 1. The observed splitting shown in Fig. 3 is substantially larger than the estimated splitting in (2). Since the magnitude of the splitting depends on the boundary condition at the Si-SiO_2 interface,[2] Eq. (2) is only an order-of-magnitude estimate and a more quantitative calculation is under way.

More interestingly, the observed splitting at 9° from (001) is substantially larger than the estimates derived from the Shubnikov–de Haas oscillations on (001) surfaces.[6] These results imply a strong angle dependence of the valley splitting.

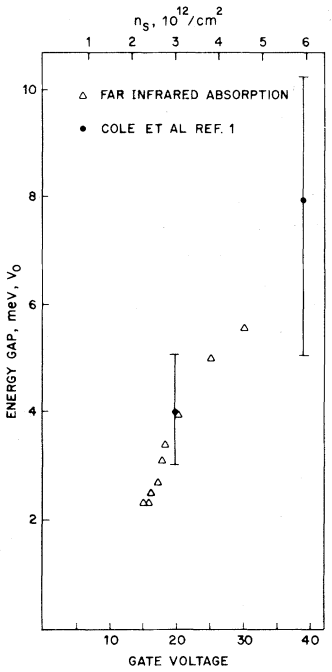

FIG. 3. Energy gap, V_0, as a function of electron density, n_s.

A more quantitative calculation based on the theory advanced here is required to check the angle dependence.

Obviously, the possible Fermi surface shapes in our model are distinguishable from the superlattice model. When the Fermi level lies above the minigap, there are, in our model, a lens orbit and a dog-bone orbit; whereas, in the superlattice model, there are the lens orbit and the open orbits.

Attempts to observe cyclotron resonance of the lens orbit have failed. Fields below magnetic breakdown,[7] ≈ 1 T, do not satisfy $\omega_c\tau > 1$ in our sample and, as expected, we have not observed the cyclotron resonance of the dog-bone orbit or of the open orbit. We note, however, that the interband structure observed at $2.5\times10^{12}/\mathrm{cm}^2$ is sensitive to magnetic fields as small as 0.5 T.

In summary, we put forward an explanation for the minigaps observed in misoriented (001) surfaces based on valley-valley splitting. The minigap is observed in the far-infrared conductivity and provides the first direct measure of the valley-valley splitting in these systems.

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