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Observation of Sixfold Valley Degeneracy in Electron Inversion Layers on Si(111)

D. C. Tsui and G. Kaminsky
Bell Laboratories, Murray Hill, New Jersey 07974

(Received 30 November 1978)

We have observed the expected sixfold valley degeneracy in the inversion layer on Si(111). This observation suggests that the twofold valley degeneracy, observed in previous experiments, cannot be an intrinsic effect due to the intervalley charge-density–wave state proposed by Kelly and Falicov.

The first quantum mechanical treatment of the electron inversion layer on (111) surfaces of Si was given by Stern and Howard,[1] using the effective-mass approximation. They predicted a sixfold valley degeneracy for the ground-state subband. (Its two-dimensional constant-energy ellipses and the first Brillouin zone are illustrated in the inset of Fig. 1.) Experimentally, however, only twofold valley degeneracy was observed in previous studies of the Shubnikov–de Haas (SdH) effect.[2-5] Kelly and Falicov[6] first proposed that this lifting of the sixfold valley degeneracy manifested a charge-density-wave (CDW) state. In this so-called CDW-β state, four of the six electron valleys were coupled, through intervalley phonon exchange interactions, into two pairs. Each pair produced one occupied bonding state, and the resulting ground-state subband was twofold degenerate. Subsequently, Nakayama[7] proposed a triple-CDW state, in which three symmetrically located electron valleys were coupled with the other three to give rise to an occupied sub-band with a twofold valley degeneracy. The formation of such intervalley CDW states has also been invoked to explain a number of anomalies observed in the inversion layers on (100) as well as (111) surfaces when uniaxial stresses were applied to the Si substrates.[8-10]

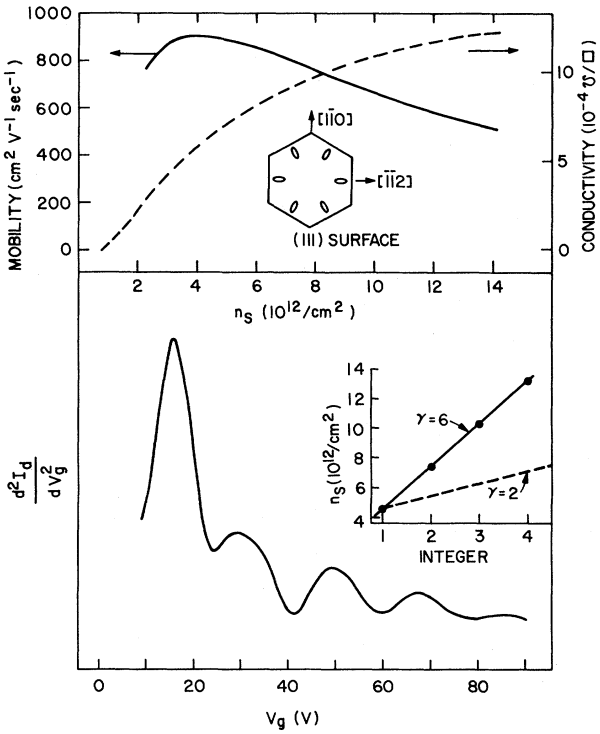

FIG. 1. Upper panel, the conductivity and mobility of an n-channel MOSFET's on (111) n-type Si at 4.2 K; lower panel, the Shubnikov–de Haas effect observed in d^2I_d/dV_g^2 as a function of V_g from the same device at 4.2 K with $B = 100$ kG applied perpendicular to the surface. The insets are explained in the text.

We have recently studied the SdH effect in a large number of n-channel metal-oxide-semiconductor field-effect transistors (MOSFET's) on the (111) surfaces of n- and p-type Si, prepared under various experimental conditions, and have observed for the first time the expected sixfold valley degeneracy in some devices. Our results suggest that the observed lifting of the sixfold valley degeneracy depends on the conditions of the Si-SiO_2 interface and that it cannot be an intrinsic effect, such as that due to the CDW state proposed by Kelly and Falicov or by Nakayama. In the rest of this paper, we shall present these results and point out that they favor an earlier model based on the existence of inhomogeneous strains at the Si-SiO_2 interface.

The experiments consist of conventional dc transport and SdH measurements on n-channel MOSFET's, fabricated on two (111)-oriented (to better 0.5°) Si wafers. One of the wafers is n type, phosphorous doped to ~ $3\times 10^{14}/\text{cm}^3$, and the other, p type, boron doped to ~ $1\times 10^{15}/\text{cm}^3$. The gate oxide was thermally grown to ~ 1400 Å in dry oxygen at 1100°C. Immediately prior to this oxidation, the wafers were annealed in argon atmosphere at 1100°C for 30 min. This argon annealing was repeated immediately after the oxidation and was subsequently followed by hydrogen annealing at 450°C for 30 min. In case of the p-type wafer, an attempt to getter dislocations[11] was made by diffusing boron into the back side before the gate oxide was grown. The gate metal was 60-Å Ti and 2000-A Al, both evaporated from sodium-free tungsten boats. The samples which we have studied include circular (Corbino geometry) and linear devices with 50-, 250-, and 400-μm channel length.

The upper panel of Fig. 1 shows the conductivity (σ) and the mobility (μ) of one sample on the n-type wafer at 4.2 K. σ was measured as a function of the gate voltage (V_g), from which the inversion-layer density (n_s) was calculated by using $n_s = C_o(V_g - V_t)/e$. Here, e is the electronic charge, V_t is the conduction threshold at 78 K, and C_o is the measured oxide capacitance per unit area. μ was calculated from $\mu = \sigma/n_s e$. The lower panel shows the SdH oscillations of this sample, observed in the second derivative of the drain current (I_d) versus V_g (i.e., d^2I_d/dV_g^2) at 100 kG and at 4.2 K. In the inset the n_s, at which dips in the d^2I_d/dV_g^2 oscillations occur, is plotted as a function of the integers designating these oscillations. The four data points lie on a straight line, as expected for two-dimensional electrons in an inversion layer. The oscillation period obtained from the slope of this line is $\Delta n = 2.9\times 10^{12}/\text{cm}^2$. This is the number of electrons induced into the channel to fill one Landau level in the ground-state sub-band. For a sub-band with a γ-fold valley degeneracy, this number is $\Delta n = 2\gamma Be/hc$, where B is the magnetic field applied perpendicular to the surface and hc/e is the quantum flux, equal to 4.14×10^{-7} G cm^2. The valley degeneracy factor, determined from our data, is $\gamma = 6.0 \pm 0.1$. Previous studies of the SdH effect gave $\gamma = 2.0$, which is indicated by the dashed line in the inset.

We have studied a total of four devices from each Si wafer. Data from accumulation layers on the n-type wafer are all similar to those shown in Fig. 1, with mobility varying from device to device by less than 10%. Data from inversion layers on the p-type wafer show ~ 30% higher mobility. However, their SdH oscillations, contrary to what might have been expected from the higher mobility, are much less pronounced, indicative of inhomogeneous smearing. In any case, we should emphasize that sixfold valley degeneracy was observed in all these devices. This observation suggests that the twofold valley degeneracy, observed in previous experiments, is not an intrinsic effect due to the CDW state proposed by Kelly and Falicov or by Nakayama. Very recently, Kelly[12] estimated the electron-electron interactions in Si and concluded that the intervalley phonon exchange interaction is too small to give rise to the CDW-β state. In addition, Beni and Rice[13] made *a priori* calculations, similar to those successfully used in the electron-hole liquid in Si. Their results show that the sixfold valley state is stable against any form of intervalley instability for $n_s \gtrsim 3\times 10^{11}/\text{cm}^2$.

These data favor an earlier model[4] based on the existence of inhomogeneous strains, resulting from the lattice mismatch at the Si-SiO_2 interface. In this model, if the strain fluctuations have predominantly long wavelengths, the interface may be pictured as divided into domains of uniaxial stresses. Within each domain the uniaxial stress lowers two of the six electron valleys to give rise to an occupied twofold valley degeneracy. Our observation of a sixfold valley degeneracy in these new samples may be understood within this model by assuming that such domains are not present in these samples. This may result from a less-strained interface. It may also be indicative of an interface where the dominant wavelengths of the strain fluctuations are shorter than the electron Fermi wavelength. Under this condition, the strain fluctuations act as electron scattering centers and the sixfold valley degeneracy is preserved. At the present, we have no direct experimental information on the condition of the interface and, thus, either explanation is plausible. In any case, several of the device-processing steps, employed in the preparation of these samples, differ from those employed for our earlier samples on which a twofold valley degeneracy was observed. These steps include the argon annealing immediately prior to growing the gate oxide (not used for earlier samples), and the use of 2000-Å Al as metal gate (instead of the 1-μm-thick Au used previously). Consequently, the interface condition of these samples is expected to differ from that of our earlier samples.

Finally, it was previously pointed out[4] that the strain required to account for the earlier observation of a twofold valley degeneracy, with n_s up to $\sim 7\times 10^{12}/\mathrm{cm}^2$, is $\gtrsim 2.6\times 10^{-3}$ (corresponding to a uniaxial stress of $\sim 5\times 10^9$ dyn/cm^2), considerably larger than that due to mismatch between the thermal expansion of Si and SiO$_2$. Recently, Feldman *et al.*[14] made helium-ion backscattering-channeling studies of the Si-SiO$_2$ interface on Si(110). They observed that the first two monolayers of Si at the interface are displaced from their bulk position by 0.1 to 1 Å, suggesting a strain from lattice mismatch of ~ 0.05 to 0.5 in the plane of the interface. Thus, if similar strain is assumed on the (111) surface, it is not difficult to visualize a strain of $\sim 3\times 10^{-3}$ in the inversion layer, which is ~ 30 Å away from the interface.

We thank S. J. Allen, A. B. Fowler, T. M. Rice, P. J. Stiles, and F. Stern for their generous comments on this work.

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Near Cancellation of Electron-Phonon Corrections in Thermoelectric Effects in Alloys

A. Vilenkin[(a)] and P. L. Taylor
Department of Physics, Case Western Reserve University, Cleveland, Ohio 44106

(Received 20 November 1978)

The corrections to the low-temperature Seebeck coefficient of dilute alloys caused by the electron-phonon renormalization of the impurity scattering vertex are found to cancel completely those other corrections due to the electron-phonon renormalization of the electron energy, velocity, and relaxation time in a model of weak s-wave scatterers, Debye phonons, and free electrons in the limit of large valence. For normal valences the electron-phonon corrections are reduced by a partial cancellation to a few percent of some recently predicted values.

The low-temperature Seebeck coefficient S of a dilute alloy has been shown by various authors in recent years to contain a number of significant terms due to electron-phonon interactions. Opsal, Thaler, and Bass[1] suggested that Prange and Kadanoff[2] had been mistaken in supposing that S was not modified by these interactions, and proposed a correction factor of $1+\gamma$, the usual electron-phonon mass enhancement correction. Following this, Lyo[3,4] found a further contribution, which in a model of weak s-wave scatterers was equivalent to a correction factor of $1+\frac{3}{2}\gamma$. In a