Spectroscopy of Valley Splitting in a Silicon/Silicon-Germanium Two-Dimensional Electron Gas

Srijit Goswami, J. L. Truitt, Charles Tahan, L. J. Klein, K. A. Slinker, D. W. van der Weide, S. N. Coppersmith, Robert Joynt, R. H. Blick, and Mark A. Eriksson

University of Wisconsin-Madison, Madison, WI 53706

J. O. Chu and P. M. Mooney
IBM Research Division, T. J. Watson Research Center, NY 10598

The strain in silicon/silicon-germanium quantum wells reduces the usual six-fold degeneracy of the silicon conduction band, leaving a pair of degenerate bands in the growth direction. Quantum confinement in the silicon well further splits this degeneracy, leading to a small, but extremely important energy gap (the valley splitting) between these lowest two levels. We perform microwave spectroscopy, electron valley resonance (EVR), between these two states. Transport measurements at 0.25 K in a silicon/silicon-germanium two dimensional electron gas are used to detect microwave absorption at the valley splitting energy. The lineshapes are similar to those observed in electrically detected electron spin resonance signals. The valley splitting is found to increase linearly with an applied perpendicular magnetic field. The valley splitting peak shows a dramatic (seven-fold) increase in width as the temperature is increased from 0.23 K to 0.35 K. These results indicate that in moderate magnetic fields the silicon valley degeneracy can be completely lifted in low temperature quantum devices.

In recent years several efforts have been made to study electron states in low dimensional systems with microwave spectroscopy. Due to the small number of electrons and low-temperature requirements, conventional microwave absorption spectroscopy techniques (which require almost \(10^{12}\) electrons for an appreciable resonance signal) are hard to employ in these structures. Therefore, transport measurements are an ideal way to probe such systems. There are a number of studies on electron spin resonance (ESR) detection in GaAs/AlGaAs two-dimensional electron gases (2DEGs) using transport measurements. However there has been only one such study in Si/SiGe 2DEGs. In addition to Zeeman splitting (in a magnetic field), strained Si structures also show valley splitting. In bulk Si the conduction band minimum is six-fold degenerate and electrons occupy six equivalent valleys. Under the influence of strain this degeneracy is lifted, resulting in a set of four-fold (higher energy) and two-fold degenerate (lower energy) valleys. As a result of quantum confinement the lowest two energy levels are split further by an energy \(\Delta_V\), the valley splitting.

Electron spins in Si are promising candidates for quantum information processing due to low spin orbit coupling. In addition, the use of isotopically pure spin zero Si-28 would eliminate decoherence due to coupling between electron and nuclear spins. For quantum computing it is highly desirable that the low lying qubit energy levels be non-degenerate. Thus it would seem that the degeneracy of valley states is a potential source of decoherence. Therefore it is vital to get an accurate estimate of the valley splitting, especially with regard to quantum computation in Si. In this Letter we show that electron transitions can be driven between the two lowest valley states using microwaves, i.e. electron valley resonance (EVR). The valley splitting is found to increase linearly with applied perpendicular magnetic field (B\(_{\text{perp}}\)). We confirm this behavior over an order of magnitude in magnetic field. Similar magnetic field dependence of the valley splitting has been seen in AlAs 2DEGs and Si-MOSFETS though over a much smaller range in B\(_{\text{perp}}\) and using different experimental techniques. Our results indicate that in moderate magnetic fields the valley degeneracy can be completely lifted, thereby suppressing a potential decoherence mechanism. We also present results on the temperature dependence of the valley splitting. We demonstrate that the EVR lineshapes are similar to those of electrically detected ESR.

The Si/SiGe heterostructure used in these experiments was grown by ultrahigh vacuum chemical vapor deposition. The 2DEG is located atop the SiGe buffer layer. The 2DEG is separated from the phosphorus donors by a 140 Å Si\(_{0.7}Ge_{0.3}\) layer, and the donors lie in a 140 Å Si\(_{0.7}Ge_{0.3}\) layer with a 35 Å Si capping layer at the surface. The [001] planes have a tilt-angle of approximately two degrees from the growth direction. Further details about the structure can be found in reference 16. The electron density of the 2DEG at 0.25 K is \(4.2 \times 10^{11}\) cm\(^{-2}\) and the mobility is 37000 cm\(^2\)/Vs. The Hall bar channel is 300 \(\mu\)m long (distance between longitudinal voltage probes) and 10 \(\mu\)m wide.

A schematic of the experimental set-up is shown in Figure 1(a). A double lock-in technique is used to measure the change in resistance, \(\Delta R_{xx}\), of the 2DEG as a function of B\(_{\text{perp}}\), in the presence of microwaves. Lock-in 1 provides bias currents ranging from 100 nA to 250 nA, modulated at 701.3 Hz. Lock-in 2 is used to estimate the valley splitting, \(\Delta R_{xx}\), in the presence of microwaves.
modulate the microwave amplitude (100% modulation) at 5.7 Hz. The output of Lock-in 1 is fed into Lock-in 2, which measures $\Delta R_{xx}$. Microwaves are produced by an HP83650A synthesizer, and are carried down to the sample using a low loss coaxial line terminated about 5 cm from the surface of the sample in a loop antenna. The base of an existing resonant cavity is replaced with a sample stage (Figure 1(b)). The microwave power at the sample has a strong frequency dependence because of the open cavity and impedance mismatches along the length of the coaxial line. Due to this non-uniformity a wide range of powers ($10^\mu$W-$10$ mW) are used to ensure sufficient delivery of power. The magnetic field is produced by a superconducting magnet and all measurements are carried out in an Oxford Instruments $^3$He cryostat with a base temperature of 0.25 K.

![Figure 1: (a) Schematic of the experimental setup, the double lock-in technique. (b) Exploded view of the open cavity used in the experiments showing the loop antenna(A) and the sample stage(S).](image)

Figure 2 shows two electrically detected ESR signals at the same microwave power (~0.5 mW). However the linewidths are slightly different due to heating effects, making it clear that the power delivery to the sample is very sensitive to the frequency. Gaussians were found to give the best fit to the curves. The plots have been normalized to set the peak height to unity. We obtain a number of such ESR signals with linewidth (extracted from the Gaussian fit) varying from 5 G to 30 G. The microwave-induced change in resistance in these signals is approximately one part in $10^4$.

The same detection scheme is used to observe EVR. Such transitions are believed to be driven by an oscillating electric field as opposed to the magnetic field, which drives spin resonance. The EVR transition amplitudes are defined by the matrix elements of the electric dipole components of the microwave field between the two valley states, which have the same spin direction in our case. The electric dipole matrix element, $V_{EV}$, is given by:

$$V_{EV} = \langle v1, \uparrow | e \mathbf{r} \cdot \mathbf{E}(r, t) | v2, \uparrow \rangle$$

$$= eE_0 \langle v1 | z | v2 \rangle \hat{e}_z = eE_0 M_z \hat{e}_z$$

where $e$ is the electronic charge, $\mathbf{E}(r, t)$ is the electric field, $v1$ and $v2$ are the final and initial valley states, $z$ is the growth direction, and $\uparrow$ denotes the spin-up state.

In the single-electron picture, the electron wavefunction in the $z$-direction of [001] strained silicon has Kohn-Luttinger oscillations (in addition to Bloch oscillations) with a period roughly determined by $k_{\text{min}}$, the distance from the Brillouin zone center to the band minimum. The rapid oscillations of the excited valley states are slightly different from the ground valley state, whereas both have the same envelope function \cite{17}. This makes $M_z$ quite small, on the order of picometers for a quantum well like the one in the sample used here \cite{18}. This implies that the electric-dipole matrix element is small, but non-zero. Nonetheless this is the dominant mechanism. The magnetic field does not induce transitions between different valley states since $v1$ and $v2$ are orthogonal, i.e. the matrix element, $V_{MV} = \langle v1, \uparrow | g \mu_B \sigma \cdot \mathbf{B}(r, t)/2 | v2, \uparrow \rangle$, vanishes. Here $g$ is the electron $g$-factor, $\mu_B$ is the Bohr magneton and $\sigma$ is the set of Pauli spin matrices. The magnetic dipole matrix element for spin resonance, $V_{MS}$, is given by $\langle \downarrow | g \mu_B \sigma \cdot \mathbf{B}(r, t)/2 | \uparrow \rangle$. It is useful to compare the magnitude of the EVR transition to the ESR
response. If we consider the ratio of the matrix elements, we find that:

$$\frac{|V_{EV}|}{|V_{MS}|} = \frac{eE_0M_z}{g\mu_B B_0/2} = \frac{eE_0M_z}{g\mu_B E_0\sqrt{\epsilon_{Si}}/c} = \frac{4mcM_z}{g\hbar\sqrt{\epsilon_{Si}}}$$

$$= (1.5 \times 10^{12} \text{ m}^{-1}) M_z \sim 1$$

where $\epsilon_{Si}$ is the dielectric constant of Si. Thus the transition amplitudes are quite comparable due to the disparity of the electric and magnetic field amplitudes i.e. $|B| = |E|\sqrt{\epsilon_{Si}}/c$. This is in good agreement with our experiments since we observe that the ESR and EVR resonances do indeed have comparable amplitudes. The current experimental set up is actually quite suitable for the detection of such electric dipole driven transitions since the sample is never at an electric field node (i.e. $E(\mathbf{r}, t) \neq 0$), thereby allowing the electric dipole matrix elements to be non-zero. We observe such valley resonances over an order of magnitude in magnetic field from about 3 T down to 0.27 T. Four such plots are shown in Figure 3. Once again, the Gaussian was found to provide the best fit for these lines. In some cases a background was subtracted off using a second degree polynomial fit. We use the same normalization procedure as for the ESR peaks. Figure 4 shows the linear dependence of valley splitting on $B_{\perp}$. This linear dependence has been observed previously over a smaller range in B in other semiconductor structures [13][14], but never in SiGe heterostructures. The microwave power dependence of the resonance peak shows a shift towards higher fields with increasing power. The largest observed shift was about 100G over two orders of magnitude in power. We use a more generous estimate of 500G for the error bars in Figure 4. A linear fit to the data gives the result $\Delta \nu \sim 1.5(\pm 0.6) + 24.7(\pm 0.4) B \text{ } \mu \text{eV}$. Since this energy scale is too small for cyclotron/spin resonance and too large for nuclear resonance, we believe that this is indeed valley splitting. Furthermore, the data is in good agreement with Koester et al. [12] who used tilted-magnetic-field Shubnikov de Haas measurements to estimate valley splitting in a Si/SiGe 2DEG. They reported a splitting of $(52 \pm 11) \text{ } \mu \text{eV}$ at $B \sim 2.7$ T, fairly close to $(68 \pm 2) \text{ } \mu \text{eV}$ measured here. Their quantum well width (10 nm) and number density $(4.8 \times 10^{11} \text{ cm}^{-2})$ are comparable to the sample used here. It has been suggested that the enhancement of the valley splitting with $B_{\perp}$ is a result of enhanced exchange interactions and electron-electron interactions [13][20][21]. However, we are not aware of the existence of a systematic theoretical explanation of a linear B-dependence. We also note that the zero field valley splitting observed here (by extrapolation) is very small, suggesting nearly degenerate valleys. Single electron calculations [17] predict much larger values for the zero-field valley splitting. A difference between this experiment and that calculation is the tilt angles in the samples used here. Ando has suggested that such a tilt can greatly suppress the valley splitting [22]. This sup-

![Figure 3](image1.png)

**FIG. 3:** Electrically detected EVR signals at four different microwave frequencies with Gaussian fits.

![Figure 4](image2.png)

**FIG. 4:** Linear dependence of the valley splitting on a perpendicular magnetic field.
pression should be less pronounced in small systems, such as quantum dots, and the valley splitting may approach the single electron value in such structures.

In conclusion, we have been able to perform microwave spectroscopy on the valley split states (EVR) for electrons in a Si/SiGe 2DEG using transport measurements. We find the splitting to be linear in B with the form: 

\[ \Delta V \sim 1.5(\pm 0.6) + 24.7(\pm 0.4)B \text{ } \mu\text{eV}. \]

The EVR technique allows measurement of the valley splitting over a wide range in magnetic field. In addition to magnetic field enhancement of the valley splitting, we also see a much smaller enhancement with increasing temperature.

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Figure 5 shows the effect of temperature on valley splitting and the resonance peak associated with it. For these measurements we choose the frequency and magnetic field associated with the largest splitting (18.11 GHz, \( \sim 3 \) T). Data sets are taken as the sample temperature is increased from 0.23 K to 0.35 K and decreased back to 0.23 K at a slow rate, giving the sample enough time to equilibrate. Error bars for Figure 5 are obtained from the hysteresis in peak widths over this up-down cycle. Even over this narrow range there is a rapid (approximately seven-fold) increase in the linewidth. This dramatic behavior suggests that it would be hard to observe such resonances at higher temperatures. In addition to thermal broadening, we observe about a 400 G (1.5%) shift in the peak position to higher fields. We conclude from this small but reproducible shift that there is also some enhancement of the valley splitting with temperature.

**FIG. 5:** (a) EVR signals from 230 mK to 350 mK with Gaussian fits. All signals have been normalized by setting the signal height at 230 mK to unity. (b) Temperature dependence of the EVR peak position. (c) Temperature dependence of the EVR linewidth.

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