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Effect of Inversion Symmetry on the Band Structure of Semiconductor Heterostructures

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Two classes of artificial semiconductor heterostructures, differing only in the inversion symmetry of their internal quantum wells, are studied via magnetotransport. The samples consist of GaAs/(AlGa)As layered structures containing two-dimensional hole systems. The results reveal a lifting of the spin degeneracy of the lowest hole subband in the samples with inversion *asymmetric* quantum wells. In those structures with *symmetric* wells the subband remains doubly degenerate.

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The concept of inversion symmetry plays an important role in solid state physics. It is one of the factors determining the degeneracies of the energy bands away from the high-symmetry points of the Brillouin zone.[1] In elemental semiconductors like germanium, with inversion-symmetric diamond structures, the heavy and light hole bands are doubly spin degenerate. In compound semiconductors (e.g., CdTe), each of these bands is split by the crystalline electric field of the nonsymmetric zinc-blende lattice. Such symmetry considerations are also expected to be of importance for artificial semiconductor superlattices.[2] In these materials, microscopic internal fields can be created and tailored to experiment.

In this paper we present a comparative magnetotransport study of two different artificial structures, each containing a two-dimensional hole system. These structures, while made from the same materials, differ fundamentally in this symmetry aspect and show directly its influence on the band structure.

By use of molecular-beam epitaxy (MBE), one-dimensional potential wells in GaAs/(AlGa)As structures were created which in one case had a symmetric, roughly square-well shape and, in the other, were roughly triangular and therefore asymmetric (see the insets to Fig. 1). Although these semiconductors are intrinsically inversion asymmetric, the resultant splittings are extremely small and can be neglected here. The potential wells, present in the valence band of the GaAs, are occupied by a degenerate two-dimensional hole system in the plane perpendicular to the well. In both cases only the lowest hole subband is populated. Though the effects described in this paper are also present in the conduction band, the heavier mass and larger spin-orbit couplings of the holes enhance the splittings.

The effect of the different symmetry on the band structure has been studied with standard magnetotransport methods. Our results show that the spin degeneracy of the lowest hole subband is lifted by the lack of inversion symmetry in the triangular well but remains intact in the symmetric square-well structure. These observations have been made with several other samples and while the quantitative data vary, the qualitative influence of inversion symmetry does not.

The samples were prepared with use of MBE as described elsewhere.[3] The triangular well consisted of a modulation-doped GaAs/(AlGa)As single-interface structure. The square-well potential was

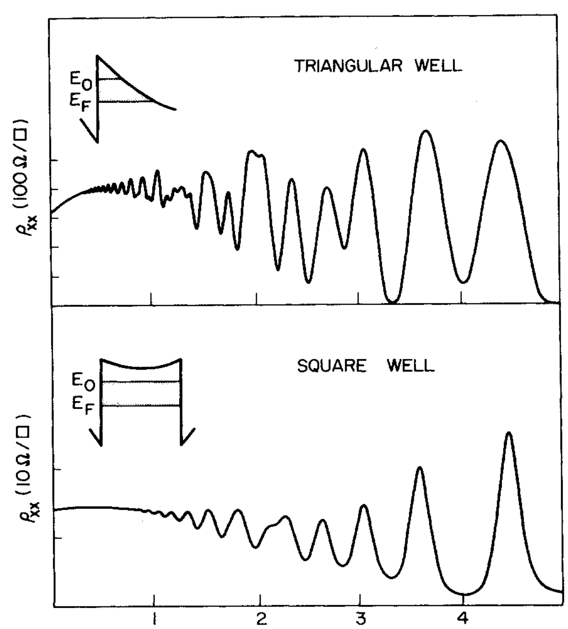

FIG. 1. Diagonal resistivity ρ_{xx} (Shubnikov–de Haas effect) of samples described in text. Insets depict variation of valence-band potential wells perpendicular to 2D plane. E_0 and E_F refer to the lowest subband and Fermi energies, respectively.

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TABLE I. Structural and two-dimensional carrier parameters for both heterostructure samples. Both structures were grown on Cr-doped GaAs substrates.

Well shape	GaAs well[a] (Å)	Spacer (Å)	(AlGa)As[b] Doped layer (Å)	Al conc. (%)	Periods	Low-T mobility [$m^2/(V/s)$]	2D density (cm^{-2})
Triangular	· · ·	120	410	48	1	3.9	4.8×10^{11}
Square	94	250	43	45	20	5.5	4.7×10^{11}

[a]Buffer; 1 μm.

[b]Dopant; Be 2×10^{18} cm^{-3}.

symmetrized by joining two equal, but opposite, interfaces together. To improve homogeneity, twenty identical, but well-separated, layers were stacked. The structural parameters for both samples are given in Table I. Shubnikov–de Haas (SdH) and Hall-effect measurements were performed on standard Hall bar geometries with diffused In/Zn contacts. A dilution refrigerator cooled the samples to 0.1 K in magnetic fields of up to 9 T perpendicular to the two-dimensional (2D) plane.

Figure 1 shows SdH results for both samples. The data between 5 and 9 T show simple periodicity in $1/B$ and are not included in the figure. For quantitative analysis, the indexed extrema in the SdH patterns are plotted versus $1/B$ in Fig. 2. Since at sufficiently high fields all Landau levels are resolved[4] and, independent of their energies, carry a degeneracy eB/h, the high-field slopes in Fig. 2 define directly the carrier densities. These are listed in Table I. Passing to lower fields, both samples show a change in the SdH periodicity in $1/B$. For the square well this break, at 2.2 T, is relatively abrupt, whereas the slope change in the triangular-well sample occurs over a broad range in which the SdH pattern shows beating. The ratio of the high- to low-field slopes in Fig. 2 is very nearly 2.0 for the square well, while for the triangular well, the ratio is 3.4. This difference is the essential point of our argument.

Two other features of the SdH data are significant here. First, from the temperature dependence of the low-field oscillations an effective mass can be determined[5]; these results are shown in Fig. 3. The square-well mass is considerably larger than that found in the triangular well. Secondly, at fields below the onset of oscillations, the triangular well has substantial positive magnetoresistance, while for the square well, this effect is much smaller.

These disparities between samples are due to the inversion symmetry or asymmetry of the associated potential wells. In the triangular well the asymmetric electric field confining the carriers to the interface is seen, in the carrier's rest frame, as an effective magnetic field lying in the 2D plane, and as being perpendicular to the wave vector $\vec{k}$. This internal field, present even in the absence of an external magnetic field, lifts the twofold spin degeneracy of the subband, thereby generating two carriers species with different masses. In the square-well sample the electric field is symmetric, and therefore the band remains doubly degenerate

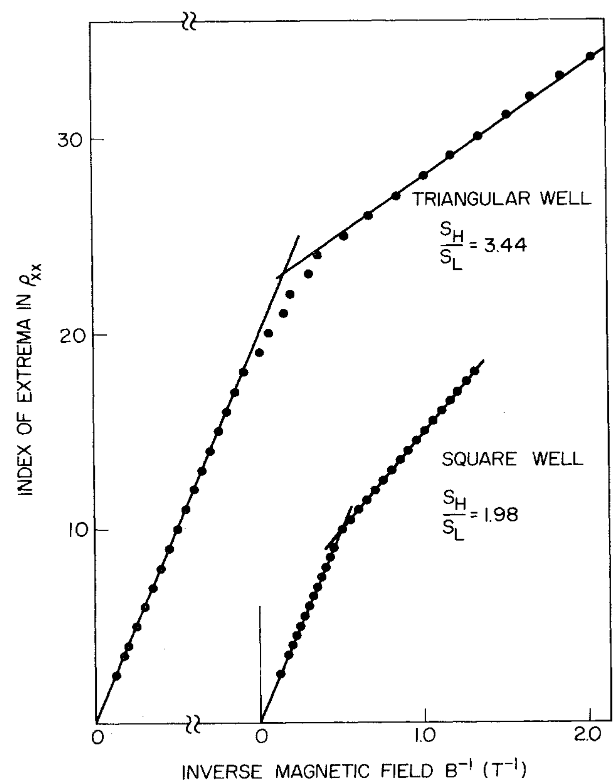

FIG. 2. Indexed extrema of ρ_{xx} vs $1/B$. Integral indices correspond to minima in ρ_{xx}, half-odd-integral to maxima. The symbols S_L and S_H refer to the low- and high-field slopes, respectively. Note the horizontal shift of origins.

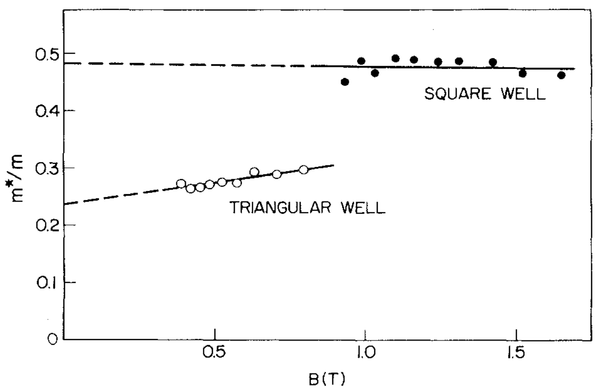

FIG. 3. Effective masses as determined from temperature dependence of SdH amplitude. For the triangular well, at low fields only the lighter mass is resolved.

with a single effective mass.

The presence of two carriers is reflected directly in the SdH data. At low field, where the oscillations first develop, only the lighter species, having a larger splitting, is resolved. Hence, the low-field slope S_L of the plot in Fig. 2 gives the population n_- of the lighter species, $n_- = eS_L/h$. At high fields, with the heavier mass also resolved, the slope S_H determines the total population $n = n_+ + n_- = eS_H/h$. Thus $S_H/S_L = 1 + n_+/n_-$; the extent to which S_H/S_L differs from 2 determines the inequality of n_+ and n_-. The linearity of the low-field plots in Fig. 2 suggests that these relative populations are field independent, and thus the ratio n_+/n_- gives an important clue to the band structure in zero magnetic field. If the spin degeneracy is lifted for finite $\vec{k}$, then the occupied areas in $\vec{k}$ space defined by the intersection of the Fermi energy with the split bands will be unequal. These areas are a direct measure of n_+ and n_-, independent of a nonparabolicity and/or anisotropy in the bands. Hence, the value $n_+/n_- \sim 2.4$ for the triangular well implies substantial splitting of the subband even in the absence of an external magnetic field. For the square well, by contrast, $n_+/n_- = 0.98$ suggests little or, within our experimental error, no lifting of the spin degeneracy at zero field.

In this framework, the observed SdH patterns find a natural explanation. The two masses arising in the triangular-well sample generate independent sets of Landau levels. At low fields only the lighter mass is resolved, but at high fields both are resolved. In the transition region the oscillations from both carriers lead to a beating pattern familiar from magnetoresistance studies of bulk zinc-blende materials.[6] For the square well the picture is simpler. Only one mass exists and the slope ratio of 2 reflects the resolution of the ordinary spin splitting of the levels induced by the external magnetic field alone. This slope transition lacks the beating effect since the magnetic field produces two sets of spin levels which simply alternate.

Possible nonparabolicity and band anisotropy make it difficult to quantitatively determine the splittings. Theoretical calculations[7-10] of the valance-band structure predict both effects to be substantial. Nevertheless, the average Fermi wave vectors of the bands follow directly from their populations. For the triangular well, we find $k_F = 1.32 \times 10^6$ and 2.07×10^6 cm^{-1} for the lighter and heavier holes, respectively. The twofold spin degeneracy of the square-well bands implies $k_F = 1.72 \times 10^6$ cm^{-1}. A further approximation is to assume parabolic bands. In this case, the population ratio n_+/n_- actually equals the ratio of the masses of the two carrier types m_+/m_-. From the mass data on the triangular well in Fig. 3, we estimate $m_- \sim 0.24 m_0$ at zero field, and thus obtain $m_+ \sim 0.59 m_0$. The square-well mass of $0.48 m_0$ fits neatly between these values, as one would expect from a spin splitting roughly symmetric about the original dispersion relation.

A final observation concerns the low-field magnetoresistance in both samples. In the triangular-well data, the large ($\sim 15\%$) positive magnetoresistance at low fields is similar to that associated with classical two-carrier conduction. In fact, fits to the data can be made with parameters not unlike those determined from the SdH slopes. The small magnetoresistance seen in the square well supports the single-carrier interpretation. However, at present we cannot rule out that spurious parallel conducting channels are contributing to the magnetoresistance.

In summary, we have demonstrated the fundamental influence of inversion symmetry of a one-dimensional potential on the band structure of artificial semiconductor structures. A triangular potential well, lacking inversion symmetry, lifts the spin degeneracy of the lowest subband in the vicinity of the Γ point of the Brillouin zone, while a square well, being symmetric, maintains a doubly degenerate band.

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[1]See, for example, C. Kittel, *Quantum Theory of Solids* (Wiley, New York, 1963).

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