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Uniaxial stress effects on a $Si/Si_{1-x}Ge_x$ double-barrier resonant tunnelling structure studied by magnetotunnelling spectroscopy

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Abstract

Magnetotunnelling spectroscopy combined with the application of uniaxial stress has been performed on a p-type $Si/Si_{1-x}Ge_x$ double barrier resonant tunnelling structure. Large effects of the strain are seen both in the intensity of the resonances, in the position of the resonance voltages, and on the curvature of the hole-subband dispersions. The change in intensity is indicative of the bandmixing taking place in the barriers. The observed voltage shifts cannot be explained by a simple four-band model for an isolated quantum well.

The large built-in strain is one of the most prominent features of $Si/Si_{1-x}Ge_x$ heterostructures. In the conduction band, a large, usable offset is only present in the case of strained Si-layers, where the two-fold degenerate Δ-minima are pushed down well below the conduction band minima in the $Si_{1-x}Ge_x$ layers. In the valence band, the built-in strain lifts the degeneracy of the light-hole and heavy-hole bands: in alloys with compressive strain, the heavy-hole states are at the valence band edge, whereas in the case of tensile strain, the band edge consists of light-hole states. Thus, the electronic and optical properties of the heterostructures are largely affected by the strain, and it is important to understand its exact role. Uniaxial stress measurements offer the possibility of changing the strain in-situ, which enables continuous tuning of the band-alignment without having to rely on samples grown on different buffer layers. Already used for early measurements of the Si valence band parameters [1], the technique was recently employed in conjunction with photoluminescence spectroscopy, to determine the type of conduction band alignment in an unstrained Si/strained $Si_{1-x}Ge_x$/unstrained Si quantum well [2]. However, to our knowledge, the valence band quantum well structure in $Si/Si_{1-x}Ge_x$ has not yet been explored with uniaxial stress.

Magnetotunnelling spectroscopy has shown itself to be a very powerful tool for the investigation of valence band structures [3]. A double-barrier resonant tunnelling structure (DBTRS) is placed in a magnetic field perpendicular to the current direction. The magnetic field will add to the in-plane momentum k_p of the carriers, so that they will tunnel through states in the quantum well with non-zero $k_p = qB\Delta z/\hbar$ (where Δz is the tunnelling distance),

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making it possible to directly probe the subbands. This has been used extensively to study p-type $S/Si_{1-x}Ge_x$ DBTRS, providing insight into the complex anisotropic and non-parabolic valence band structure [4]. Nevertheless, there are still many unanswered questions into the nature of the bandmixing effects taking place in the tunnelling mechanism. It is clear that these must be important: the emitter of the DBTRS consists of heavy holes, whereas clear resonances also from light-hole states can be seen in the I–V characteristics. Here, we combine the magnetotunnelling with uniaxial stress, to gain further insight into the conduction mechanism in these structures.

The p-$Si/Si_{1-x}Ge_x$ DBTRS were grown on (100)-substrates using atmospheric pressure CVD. The details of the growth can be found in Ref. [5]. They consist of a 46 Å wide, strained $Si_{0.75}Ge_{0.25}$ quantum well surrounded by 50 Å wide, unstrained Si barriers, and graded $Si_{1-x}Ge_x$ emitter and collector regions. The I–V characteristics at $T = 4.2$ K show three resonances, corresponding to three subbands in the quantum well: HH0 (37 meV from the heavy-hole valence band edge), LH0 (91 meV), and HH1 (138 meV). The heavy-hole and light-hole potentials are separated by ≈ 46 meV, so that, at low temperatures the emitter is only populated by carriers in the heavy-hole states. These heavy holes tunnel through both the heavy-hole and light-hole subbands in the quantum well. Using a self-consistent calculation for the bandprofile, the resonant voltages correspond well to the energy-values of the quantum well states.

Long slivers (≈ 1.5 cm) of the wafer were cut along the easy cleavage planes {111}, with mesa structures of the DBRTS at one end. A beam-bending technique [6] was employed to apply a uniaxial stress along the (110) direction perpendicular to the growth direction, and along the long axis of the sliver. The end close to the mesa structures was clamped in a copper block, while the free end was put into the slot of a comb-like block, that could carefully be moved perpendicular to the beam axis, thus bending the silicon sliver. As the mesa height is much smaller than the thickness of the sliver, the double barrier structure will essentially follow the surface of the beam, making both compressive ($S < 0$) and tensile stresses ($S > 0$) possible. The maximum stress thus obtained, before breaking the sample, was $\approx \pm 1.8$ kbar. The sample was put into a magnetic field parallel to the stress axis, and I–V and dI/dV–V characteristics were measured at $T = 4.2$ K and in fields up to 15 T, using standard lock-in techniques.

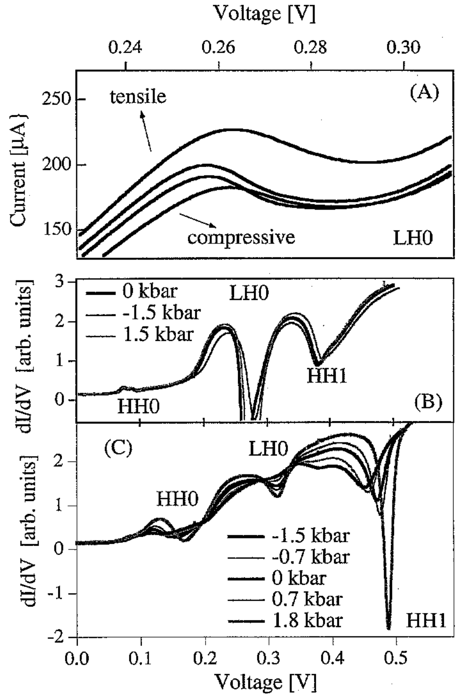

Fig. 1. I–V and dI/dV–V characteristics for the DBRTS at $B = 0$ T ((A) and (B)) and at 15 T, for different applied uniaxial stresses. Tensile stress is defined as positive. In (A), from top to bottom, $S = 1.8$ kbar, 0.7 kbar, 0 kbar, and -0.7 kbar. Please note that (A), (B) and (C) have different voltage scales.

In Fig. 1 the conductance versus voltage is shown for different applied stress, at $B = 0$ T and $B = 15$ T. The resonances are identified according to the calculations of the well levels for $k_p = 0$. At zero magnetic field, no or very small stress shifts are seen for the two heavy-hole resonances. The HH1 resonance in the I–V curve becomes slightly more accentuated for compressive strain. On the other hand, the light-hole resonances move towards higher voltages for both compressive and tensile stress, and the peak current is increasing for compressive strain, while the valley current remains fairly constant. The changes in the characteristics are more apparent at

$B = 15$ T. Both heavy holes are moving towards higher voltages for tensile stress, whereas the light-hole resonance moves in the opposite direction. However, all three resonances become deeper for tensile stress. The change is quite significant, as is seen, for example, in the HH1 resonance, which is only seen as a minimum in the conductance for $S \geq 0$, but develops negative differential resistance for $S < 0$. One also notes, that the two heavy-hole resonances seems to develop a split structure for compressive strain.

Care must be taken, that the observed changes really correspond to changes in the double barrier structure, and are not due to strain-induced changes in the resistance of the contact layers, of the development of dislocations in the (already) highly strained $Si_{1-x}Ge_x$ layers, or simply a deterioration of the ohmic contacts. For several reasons we exclude these possibilities: (A) The changes are reversible, as observed when passing from tensile to compressive and back to tensile stress again. (B) The contact layers are degenerately doped ($p = 10^{-19}$ cm^{-3}). Any changes in the resistance of the contact layers would therefore be negligible compared to the total resistance of the structure. (C) Models with additional series resistances (or parallel resistances) are not able to transform the I–V curves for different applied stress into each other. (D) The fact that the HH and the LH resonances move in different directions indicates the non-linear nature of the effects, and it is therefore reasonable to assume, that indeed, it is the double barrier structure that is responsible for the shifts

In Fig. 2, the shift of the different voltage resonances is shown as a function of strain, for the two cases, $B = 0$ T and $B = 15$ T, respectively. Using the self-consistent calculations of the bandprofile, one finds that, except for the lowest voltages (< 100 mV), the applied shift in energy of the centre of the quantum well with respect to the emitter Fermi energy is roughly proportional to the applied bias. At high magnetic field both heavy-hole resonances shift almost linearly with the strain, with a coefficient $dV_{HH}/dS = -10$ mV/kbar ≈ 3 meV/kbar. For $B = 0$ T the corresponding $|dV_{HH}/dS|$ are less than 1 mV/kbar. The LH0 displays a U-shaped curve at $B = 0$ T, with a change in energy of ≈ 5 meV at $S = 1.4$ kbar, and ≈ 1.5 meV at $S = -1.7$ kbar. The

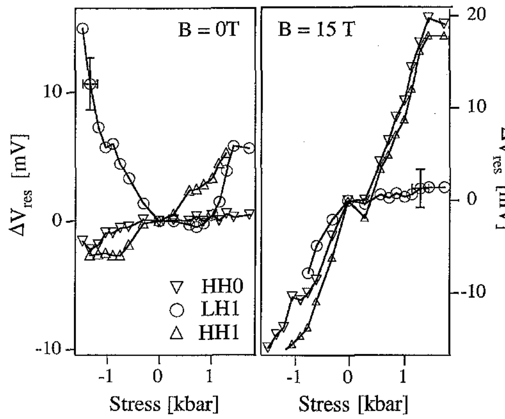

Fig. 2. The observed stress-induced shifts of the resonant voltages for $B = 0$ T and $B = 15$ T. The curves are connected as a guide for the eye. Typical error bars are shown in the figure.

change in resonance voltage for compressive strain at 15 T is uncertain as the resonance is rather weak in this region, making the exact determination of the resonance voltage difficult. However, the strain-induced shifts at 0 T and 15 T give a far from complete picture, and it is necessary to study the experimental dispersion relations to fully capture the effects of the uniaxial stress on the light-hole resonance. In Fig. 3 the resonance voltages versus magnetic field are shown for $S = -1.5$ kbar, 0 kbar, and 1.5 kbar. On the righthand scale we have included the corresponding energy scale. Here, the LH0 dis-

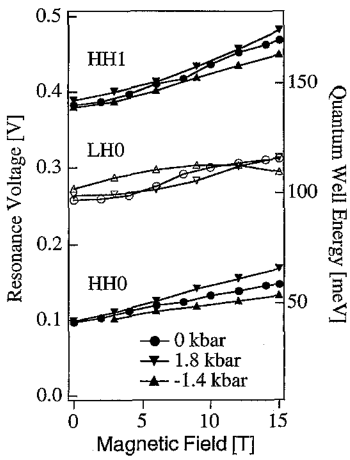

Fig. 3. Measured dispersion relations for the three resonances, for $S = 0$ kbar, 1.8 kbar, and -1.4 kbar.

plays a strain-induced transition, from a positive to a negative in-plane effective mass.

The changes in intensity of the different resonances may be explained by the mixing of the wavefunction that occurs in the barrier as the emitter heavy holes tunnel through to the quantum well states. Under tensile uniaxial stress, the light-hole barrier will be lower than the heavy-hole barrier (and vice versa for compressive stress). As in the case of crossover between Γ and X-barriers in a n-type GaAs/AlGaAs DBRTS [7], one would expect the carriers to see mainly the lowest barrier, and, in the case of tensile stress, they would be expected to obtain a small but increasing light-hole character. At $B = 0$ T, this would increase the tunnelling probability into the light-hole state, and decrease it for the heavy-hole state, as is indeed observed. At $B = 15$ T, the holes tunnel into states with a significant in-plane momentum, which are no longer pure heavy- or light-hole states. The barrier-induced band-mixing therefore leads to an increase of the strength of all the resonances under tensile stress.

Calculations of the hole-subbands in a $Si/Si_{1-x}Ge_x$ quantum well have been performed, in order to compare with the experimentally observed voltage resonance shifts. For simplicity, only the heavy-hole and light-hole bands were taken into account, and the barriers were assumed to be infinitely thick. To the usual Luttinger Hamiltonian a strain Hamiltonian is added, given by [1]

$$H_e = \tfrac{2}{3}D_u\left(\left(J_x^2 - \tfrac{1}{3}J^2\right)e_{xx} + \text{c.p.}\right) + \tfrac{2}{3}D'_u\left(\{J_x, J_y\}e_{xy} + \text{c.p.}\right), \tag{1}$$

where $\{J_i, J_j\}$ is the anticommutator, c.p. are cyclical permutations of the terms, and the strain tensor e is given by Hooke's law: $e_{ij} = s_{ijkl}S_{kl}$, where s_{ijkl} are the elastic constants. A linear interpolation between Si and Ge was used to obtain the material constants of the $Si_{0.75}Ge_{0.25}$-alloy. This is expected to be a reasonable approximation for the range of Ge-content in the different layers. The analytical solutions for the bulk wavefunctions, together with the usual boundary conditions for a quantum well, were used to calculate the energies of the subbands [8]. The result for three different levels of stress are shown in Fig. 4. The energies are given from the top of the $Si_{0.75}Ge_{0.25}$ valence band (including strain), in absolute values. The general behaviour of the subband dispersions agrees with the observed resonances. Furthermore, some of the experimentally seen strain-dependencies are indeed manifest in the calculated subbands. At $k_p = 0$ ($B = 0$), the HH-resonances do not shift. This is also what would be expected, since the holes will tunnel from heavy-hole states in the emitter, with no relative energy shift between the emitter and quantum well states (ignoring the slight difference in the elastic constants of Si and $Si_{0.75}Ge_{0.25}$). A closer inspection of the LH0 subband shows, that its curvature is indeed sensitive to the uniaxial stress, with a compressive stress leading to a negative curvature (in absolute energy).

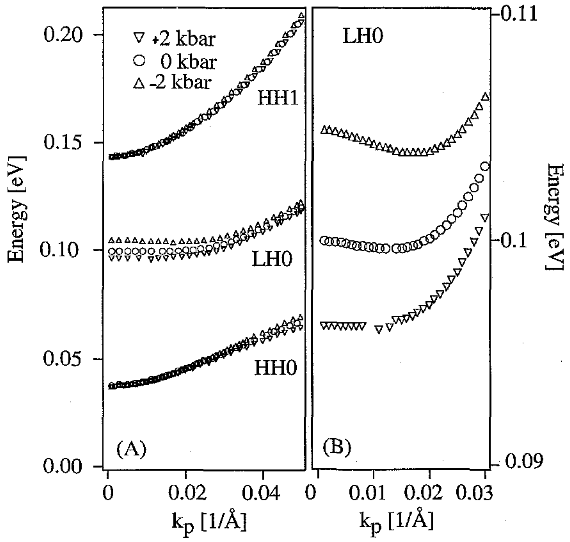

Fig. 4. Calculated subband dispersions for the three lowest subbands in the $Si_{0.75}Ge_{0.25}$-quantum well, for uniaxial stress $S = -2$ kbar, 0 kbar, and 2 kbar. The band offset has been assumed to be ≈ 223 meV, and the LH–HH separation (at zero uniaxial stress) ≈ 24 meV. (B) shows a zoom of the LH0 resonance, indicating a transition from positive to negative in-plane effective mass.

However, there are significant qualitative differences between the measured and calculated resonance energies, most notably at high in-plane momenta (or high B), where only small shifts of the heavy-hole resonances to *higher* energies for compressive strain are seen, compared with the fairly large linear shift to *lower* resonance voltages observed. The calculated shifts are also what one would intuitively expect: a tensile stress reduces the split between the heavy-hole and light-hole potential, so that the higher LH subbands will repel the HH subbands, resulting in a smaller dispersion. Nor does the U-shaped curve of the LH0-shift at 0 T correspond to the quite large, linear shift seen in the calculated subband at $k_p = 0$. The calculated shift is a result of lowering or raising the light-hole potential with respect to the heavy-hole bulk band, for tensile and compressive stress, respectively. The shift towards higher voltages when applying a tensile stress cannot be explained by this model.

Magnetotunnelling spectroscopy has proved itself very useful in the study of hole-subbands in GaAs quantum wells [3]. However, we find here that caution has to be taken when dealing with a highly strained system, such as $Si/Si_{1-x}Ge_x$, where the conduction mechanism of a DBRTS is found to be more complex. Our results indicate, that the strain is an important parameter, and that it is not sufficient to consider the effects on the well subbands in an isolated quantum well. In a more realistic model, the finite size of the barriers, the spin-split band, and any effect of band-mixing and scattering of the incoming holes have to be considered. Furthermore, the complete nature of the emitter is not taken into account. The graded region will reduce the band splitting at larger distances from the double barrier. It is conceivable, that light holes, with their lighter mass in the current direction, may play a role in the tunnelling into the light-hole state. Further experimental and theoretical studies are currently being undertaken to elucidate the hole-conduction mechanism in these $Si/Si_{1-x}Ge_x$ heterostructures.

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