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Stress and pressure effects on a Si/SiGe double-barrier structure studied by magnetotunnelling spectroscopy

P. Gassot^a, Ulf Gennser^{b,*}, D.M. Symons^a, A. Zaslavsky^c,
D.A. Grützmacher^b, J.C. Portal^{a,d}

^a Grenoble High Magnetic Field Laboratory, MPI-FKF and CNRS, BP 166, F-38042 Grenoble CEDEX 9, France

^b Paul Scherrer Institute, CH-5232 Villigen PSI, Switzerland

^c Division of Engineering, Brown University, Box D, Providence, RI 02912, USA

^d INSA-Toulouse, 31077, France

Abstract

Si/SiGe double-barrier resonant tunnelling structures have been studied using magnetotunnelling spectroscopy while applying either uniaxial stress or hydrostatic pressure. The stress dependence of some of the observed resonances indicate that the $dI/dV-V$ characteristics cannot simply be explained by tunnelling of the emitter heavy-holes through heavy-hole or light-hole quantum well subbands at different points in k -space. Instead, scattering in the light-hole-like barrier seems to be of importance. © 1998 Elsevier Science B.V. All rights reserved.

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The valence band is of special interest in Si/SiGe heterostructures, since in fully pseudomorphic structures grown on Si substrates the conduction band offset is too small to be of practical use. The valence band offset has been used extensively in studies of, e.g., two-dimensional hole gases [1] and resonant tunnelling structures (RTS) [2,3]. Magnetotunnelling spectroscopy has been proven to be a very useful tool for studying the complex valence band structure, and specifically, to probe the

subband dispersion curves of the valence band quantum well in a RTS. A magnetic field applied perpendicular to the current direction add to the in-plane momentum k_p of the carriers, so that they tunnel through states in the quantum well with non-zero $k_p = qB\Delta z/\hbar$ (where Δz is the tunnelling distance), making it possible to directly probe the subbands. However, from such experiments it has also been clear that the tunnelling through a Si/strained SiGe double-barrier structure is more complex than can be explained by tunnelling of heavy holes through the valence band quantum well subbands [4]. Here we will describe resonant tunnelling experiments that use uniaxial stress and hydrostatic pressure as a small external

* Corresponding author. Tel.: + 41 56 310 2839; fax: + 41 56 310 2646; e-mail: gennser@psi.ch.

perturbation, in order to understand the transport mechanism of holes in this highly strained system.

The effect of a uniaxial stress is to lift the degeneracy at the Γ point between the light-hole and heavy-hole bands. In a pseudomorphically grown, strained SiGe alloy the built-in biaxial, compressive strain has already broken the symmetry between the in-plane directions and the direction parallel to the growth direction, with a result of lowering the light-hole band below the heavy-hole band edge by ca. 8 meV/%Ge in the alloy. A uniaxial stress either slightly reduces the band splitting (tensile stress) or increases it (compressive stress). In the RTS, the Si barriers will be unstrained. In these pure Si layers, the externally applied stress will by itself lift the degeneracy between the light and heavy holes. On the other hand, a hydrostatic pressure does not break the symmetry, and a priori would not be expected to affect the relative position of the valence bands, and therefore not the transport properties of a RTS. However, as has been shown in absorption measurements on GaInAs/AlInAs multiple quantum wells, a hydrostatic pressure applied on a heterostructure can lead to an effective biaxial strain due to the different elastic constants of the constituent materials [5]. The difference between the hydrostatic pressure and an externally applied uniaxial stress over all layers is that only the SiGe layers will experience a tensile stress. This difference is utilised to distinguish between different tunnelling paths through the Si/SiGe RTS.

The p-Si/Si_{1-x}Ge_x RTS were grown on (1 0 0)-substrates using atmospheric pressure CVD. The details of the growth can be found in Ref. [6]. They consist of a 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 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 (HH) and light-hole (LH) subbands in the quantum well. Resonances observed in the I - V characteristics at $T = 4.2$ K show the expected confinement shift for samples with different well widths. Two different samples were used in the pressure measurements, with a 35 and 46 Å quantum well, respectively. The results from the two

samples are qualitatively similar, and in the following only the results of the 46 Å quantum well sample is shown. A beam-bending technique [7] was employed to apply both compressive ($S < 0$) and tensile uniaxial stress ($S > 0$) along the (1 1 0) direction perpendicular to the growth direction. The maximum stress thus obtained, before breaking the sample, was $\approx \pm 1.8$ kbar. For the hydrostatic pressure experiments ($p \leq 7.5$ kbar), the sample was mounted in a liquid clamp pressure cell. I - V and dI/dV - V characteristics were measured at $T = 4.2$ K and in magnetic fields ($B \leq 15$ T) perpendicular to the current, and (in the case of uniaxial stress) parallel to the stress axis.

The dI/dV - V characteristics of the 46 Å well sample reveals three resonances. Self-consistent calculations for the band profile shows that the observed resonant voltages correspond well to the three subbands in the quantum well: HH0 (37 meV from the heavy hole valence band edge), LH0 (91 meV), and HH1 (138 meV). All three resonances shift to higher fields when a magnetic field is applied perpendicular to the current direction. The curves obtained when plotting the RTS resonance voltages versus magnetic field has been interpreted as mapping out the dispersion curves $E(k)$ of the non-parabolic quantum well subbands [8,2]. Theoretical investigations have shown this picture to hold as long as the quantum well is not too wide [9].

The externally applied uniaxial stress leads to shifts in the resonance voltages (see Fig. 1), which especially at high magnetic fields can be of the same magnitude as the shifts induced by the B -field itself. This is expected: the in-plane kinetic energy at 15 T is ≈ 7 meV (assuming a parabolic dispersion, an effective hole mass of $0.3 m^*$, and a tunnelling distance of 100 Å), whereas the reduction of the splitting between the heavy and light hole bands at $S = 1.8$ kbar is ≈ 4 meV. However, even qualitatively some of the observed uniaxial stress-induced shifts do not agree with the dispersion relation picture. This is especially true for the two heavy-hole resonances: at zero magnetic field very small shifts are expected, since the relative position between the heavy-hole emitter state and the heavy-hole quantum well potential does not change with the stress. At high magnetic fields, the heavy-hole

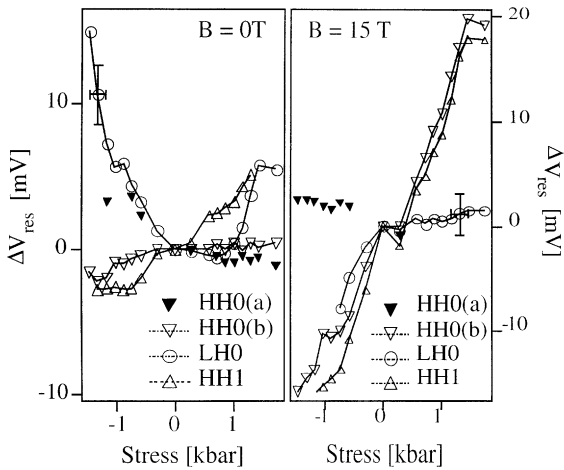


Fig. 1. The observed uniaxial stress-induced shifts of the resonant voltages for $B = 0$ and 15 T. The larger HH0 resonance is labelled HH0(b). The shifts for the smaller HH0(a) resonance are taken at 12 T, since the resonance can only be seen for the highest compressive strains at 15 T. The curves are connected as a guide for the eye. Typical error bars are shown in the figure.

subbands will attain some light-hole character, and a tensile stress would therefore be expected to lead to a lowering of the HH resonance voltages, since the band splitting is reduced. Instead, a fairly linear shift to higher voltages for tensile stress, and to lower voltages for compressive stress, is seen. The situation for the LH resonance is somewhat more complicated, since its position between the two HH-resonances leads to a large amount of band mixing. Here, a compressive strain leads to an inversion of the curvature, and a negative effective mass, which is also predicted by calculations of the subband dispersions [4].

The uniaxial stress also reveals a splitting of the HH resonances. In Fig. 2 the $dI/dV-V$ curve for the HH0 resonances is shown for $B = 15$ T and different uniaxial stress. A weaker resonance appears below each of the main HH resonances when the sample is strained compressively. It gets fainter as a tensile stress is applied, and can then only be seen at lower magnetic fields. The second HH1 resonance is only visible at the highest compressive strains and magnetic fields. The two HH0 resonances have been studied in detail for $S = 0$ (Fig. 3). The higher of the two shows a very clear linear

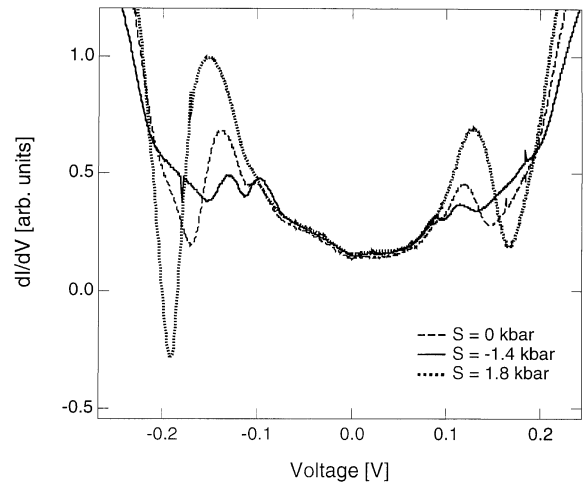


Fig. 2. $dI/dV-V$ characteristics of the RTS for different uniaxial strains, scanning through the HH0 resonances for both forward and reverse bias at $B = 15$ T.

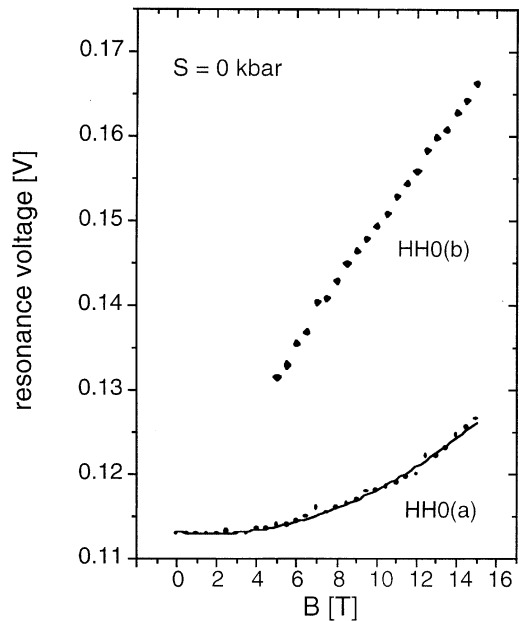


Fig. 3. Magnetic field shift of the two HH0 resonances at $S = 0$ kbar. The full line is a quadratic fit of the HH0(a) resonance.

dependence on the magnetic field. This linearity remains for different uniaxial strains, but the slope changes linearly with S , as can be seen in Fig. 1. The lower resonance displays a parabolic behaviour,

and little strain dependence. The behaviour is much closer to what one would expect from the tunnelling through the HH0 states, but this tunnelling path is masked by the larger, linearly dispersive resonances.

It is surprising that the rather small-energy perturbation of the uniaxial stress can have such a large effect in quenching some of the tunnelling paths. However, the tensile stress leads to a qualitative change in the barrier potential, splitting the barrier potential so that the band edge becomes light-hole like. As mentioned in the introduction, a hydrostatic pressure can lead to a uniaxial stress in the SiGe layers, but will not affect the strain in the Si barriers. Using pressures up to 7.5 kbar, it is possible also here to detect shifts in the RTS resonances. In Fig. 4 the shifts of LH0 and HH1 are shown as a function of pressure. As Ge is a softer material than Si, the SiGe layers will experience a tensile stress, as they follow the lattice period of the Si substrate. Using an interpolation between the elastic constants for Si and Ge, it is estimated that the stress thus obtained is a factor of two smaller than the tensile stress obtained in the uniaxial stress measurements, i.e. a hydrostatic pressure of 7.5 kbar corresponds roughly to a uniaxial stress of 0.9 kbar. In addition, the band gap is affected by the pressure. It is possible that

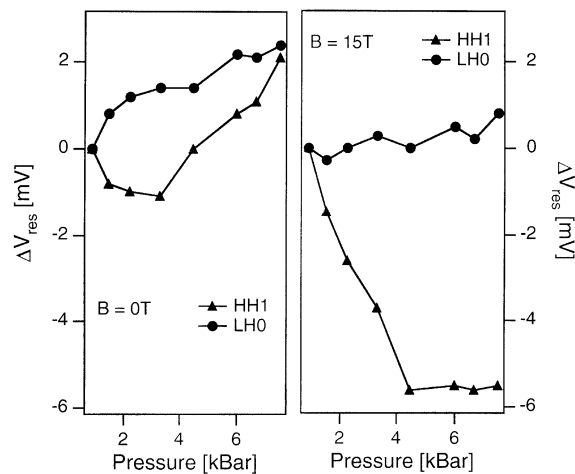


Fig. 4. The observed hydrostatic pressure-induced shifts for $B = 0$ and 15 T. The curves are connected as a guide for the eye.

a hydrostatic pressure will lead to changes in the effective masses, since they depend primarily on the direct band gap. We have not been able to find any values of the pressure coefficient of the direct band gap of Si, but using the value of Ge, it is estimated that it may lead to changes in the dispersion relations of the same magnitude as those due to the resulting tensile stress. Due to the uncertainties in these values, it is therefore difficult to compare the measurements with calculated dispersion curves. However, neither the resulting tensile stress nor the change in effective masses would lead to a lifting of the degeneracy of the barrier potential. In Fig. 5, the $dI/dV-V$ characteristics for the HH0 at $B = 15$ T are shown for different p. It is clear that there is no discernible shift, nor is there a change in the relative strength of the resonances, as is found in the characteristics using uniaxial stress.

It may here be appropriate to point out that it does not seem likely that the stronger HH0 resonance stems from a spin splitting of the quantum well state. The “heavy-hole” and “light-hole”

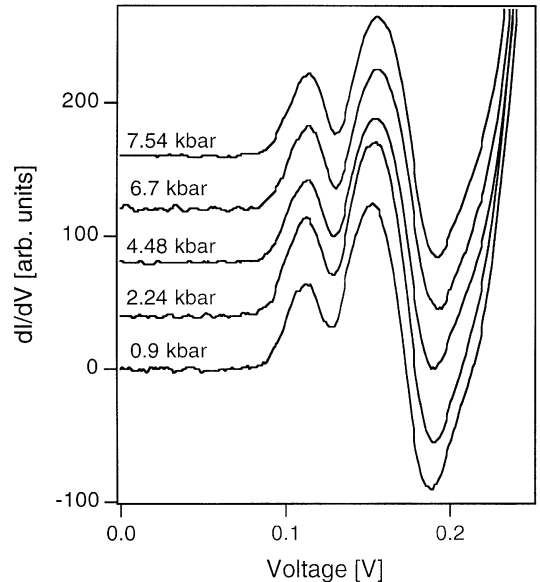


Fig. 5. $dI/dV-V$ characteristics of the RTS for different hydrostatic pressures, and at $B = 15$ T, scanning through the reverse bias HH0 resonances. The voltage axis has been inverted, and curves have been displaced for clarity; the zero-bias conductance is identical for all pressures.

description of the subbands stems from the wavefunctions for zero in-plane momenta also being eigenfunctions of the angular momentum operator J_z , where z is the direction perpendicular to the interfaces. The spin-part of the Hamiltonian for a magnetic field parallel to the interfaces has the form $H_S = -2\kappa\mu_B B J_x$, and the expectation value $\langle J_x \rangle$ is zero for a HH state at $k_p = 0$. On the other hand, if the tunnelling process goes via non-zero k_p , the HH parabolic dispersion should be added on to the resonance voltage, and the linear dependence as a function of magnetic field would not be observed. Similarly, because of the orientation of the magnetic field one would not expect any Landau level splitting of the resonances. The uniaxial stress dependence of the two HH resonances follows the shift of a LH \rightarrow HH tunnelling path, rather than a HH \rightarrow HH or HH \rightarrow LH path. This, taken together with the evidence from the hydrostatic pressure experiments, indicates that the alignment in the barrier is determinant for this process, possibly

with by scattering into LH states of the incoming HH states. However, further studies are still needed to elucidate the exact tunnelling process.

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