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# Electronic structure of [111] Si/Ge superlattices

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**Abstract.** Using *ab initio* pseudopotentials we have performed self-consistent calculations on  $\text{Si}_n/\text{Ge}_n$  strained layer superlattices grown on a (111) silicon substrate for  $n = 1, 2, 3$  and  $n = 6$ . We look at the electronic structure and find that, despite strain and folding effects, none of these superlattices have a direct gap. From charge density contours a complete localization of the upper valence band states at the  $\Gamma$  point is found on the germanium sublattice for the  $n = 6$  case. Such localization does not occur for superlattices grown on (001) substrates with the same repeat distance.

## 1. Introduction

Silicon technology centres around the (001) substrate and most theoretical [1–8] and experimental [9–12] work on Si/Ge superlattices have thus concentrated on this orientation. The principal result has been in the finding of new low-energy direct transitions [9]. This has been confirmed in many of the calculations. Froyen, Wood and Zunger [5] found that for superlattices grown on a (001) substrate the six X conduction band states split. Those perpendicular to the substrate, which fold onto the  $\Gamma$  point, move up in energy and those parallel to the substrate move down in energy. If a substrate with a larger lattice constant was used then the perpendicular bands which fold onto the  $\Gamma$  point, move down in energy giving a quasi-direct gap. They have also studied superlattices grown on a (110) silicon substrate [13] and found that the X bands which fold onto the  $\Gamma$  point are now the lower ones in energy. In this work we look at superlattices grown on a (111) silicon substrate.

## 2. Method

The calculations were done in a supercell geometry using the norm-conserving non-local pseudopotentials of Bachelet, Hamann and Schlüter [14] with the exchange–correlation potential of Hedin and Lundqvist [15]. A special points scheme [16] was used to calculate the charge density and plane waves of up to 11 Ryd were found to be necessary to give the correct ordering of conduction band levels. The atom positions in these strained systems were calculated using the inter-atomic potentials of Stillinger and Weber [17]. For [111] orientated superlattices there are two different kinds of bonds. There are bonds in the [111] direction akin to the dangling bonds of a (111) silicon surface and there are bonds oblique to the growth direction akin to the back bonds of a (111) silicon surface. For the  $n = 2$  and the  $n = 6$  superlattices the interface bond is taken as the

**Table 1.** Interplanar back bond and dangling bond distances ( $\text{\AA}$ ) for bulk silicon, germanium strained to a (111) silicon substrate and the [111]  $\text{Si}_n/\text{Ge}_n$  superlattices.

	Silicon	Strained germanium	$\text{Si}_1/\text{Ge}_1$	$\text{Si}_2/\text{Ge}_2$	$\text{Si}_3/\text{Ge}_3$	$\text{Si}_6/\text{Ge}_6$
Si-Si	0.7838 2.3510	—	—	0.7838	0.7838 2.3510	0.7838 2.3510
Si-Ge	—	—	0.8229	—	0.8671	—
	—	—	2.3843	2.3843	2.3843	2.3843
Ge-Ge	—	0.8505	—	0.9005	0.9005	0.9005
	—	2.4510	—	—	2.4343	2.4343

dangling bond of the silicon surface. The  $n = 3$  superlattice has, however, two different kinds of interface. One interface has the interface bond in the growth direction and the other has the interface bond oblique to the growth direction. We refer to the two different kinds of interface bonds as dangling bonds and back bonds respectively. The planar spacings for bulk silicon, germanium strained to a (111) silicon substrate and for the superlattices studied here are given in table 1.

In the local-density approximation (LDA) the unoccupied conduction band states are incorrectly described [18]. We, however, find that for bulk silicon and germanium the discrepancy with experiment [19] is nearly the same for all lower conduction band states. We assume, therefore, that we can correct for the superlattice by shifting the entire conduction band upwards to obtain the correct band gap. As calculated deformation potentials are in good agreement with experiment this assumption seems reasonable for a strained system.

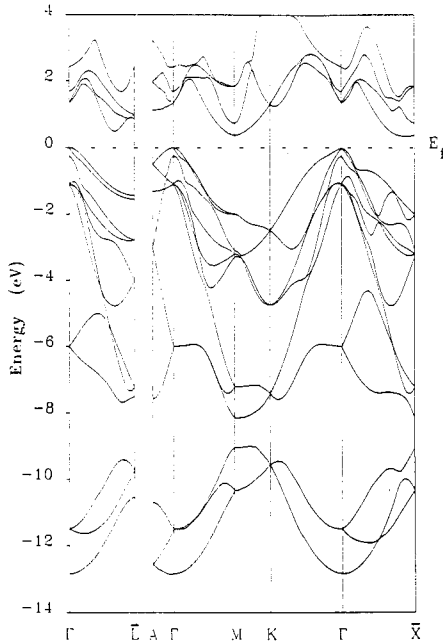
Spin-orbit splitting effects have been ignored in these calculations.

### 3. Results

#### 3.1. Electronic structure

The unit cell of this system is hexagonal. For the  $n = 1$  and  $n = 3$  superlattices we have used a six-atom unit cell with point group symmetry  $C_{3v}$  and for the  $n = 2$  and the  $n = 6$  superlattices we have used a twelve atom unit cell with point group symmetry  $D_{3d}$ . The face centre cubic (FCC)  $\Lambda$  direction becomes the  $\Delta$  direction in the hexagonal unit cell. For  $n$  even, the FCC L point in the [111] direction folds onto the hexagonal  $\Gamma$  point and for  $n$  odd the FCC L point in the [111] direction folds onto the hexagonal A point. The FCC X point is equivalent to the hexagonal M point although the symmetry directions FCC  $\Gamma\text{X}$  ( $\Delta$ ) and hexagonal  $\Gamma\text{M}$  ( $\Sigma$ ) are not. This is because the FCC X point lies in a different Brillouin zone. In the following and on all diagrams an overbar is used to indicate a FCC label.

Figure 1 shows the full band structure for the  $n = 1$  superlattice plotted in the hexagonal unit cell in which the calculation was performed with the inclusion of the FCC  $\overline{\Gamma\text{X}}$  and  $\overline{\Gamma\text{L}}$  directions. Although this unit cell is not primitive for the  $n = 1$  superlattice, 'true' states can be distinguished from 'folded in' states by an examination and comparison of charge density contours of all the systems studied here. Calculations on the  $n = 1$  superlattice in a two-atom unit cell confirm the identification of states. Under [111] strain there are two inequivalent sets of  $\overline{\text{L}}$  points. There are those in the [111] direction

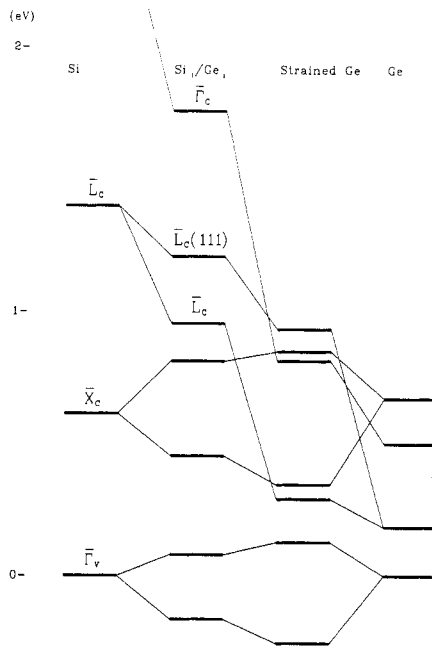


**Figure 1.** Band structure of the [111] Si<sub>1</sub>/Ge<sub>1</sub> superlattice.

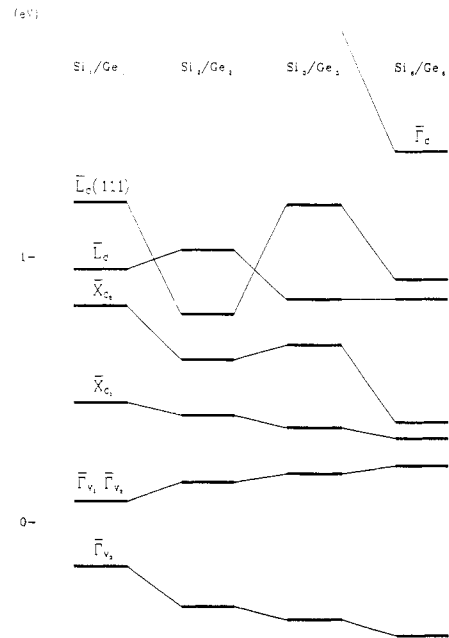
of growth which fold onto the A or  $\Gamma$  point hereafter referred to as  $\bar{L}(111)$  and those in the six directions equivalent to  $[\bar{1}11]$  hereafter referred to simply as  $\bar{L}$ . There is a gap in the valence band as in all compound semiconductors, a splitting of levels at the valence band  $\Gamma$  point due to strain and a conduction band minimum near the  $\bar{X}$  point. The folding of states onto the  $\Gamma$  point has lowered the lowest conduction band  $\Gamma$  state but it is still an indirect gap semiconductor. The figure has not been corrected for the LDA error. A uniform shift of  $0.62 \pm 0.04$  eV is required for this.

In figure 2 we plot the energy levels at symmetry points for silicon, the  $n = 1$  superlattice, germanium strained to a (111) silicon substrate and unstrained germanium. For germanium the conduction band minimum is at the  $\bar{L}$  and  $\bar{L}(111)$  points which for no strain are equivalent. The effect of strain on germanium is to split the  $\bar{L}$  and the  $\bar{L}(111)$  states. The  $\bar{L}(111)$  states move up with respect to the  $\bar{L}$  states as predicted by first order deformation potential theory [20]. However, first order deformation potential theory cannot account for the splitting of the  $\bar{X}$  states which we find and higher order terms in the theory need to be included for this. This is only to be expected as the 4% strain is outside the limit of first order deformation potential theory and the  $\bar{X}$  states have a large component in the  $\bar{L}$  direction. Recent calculations by Qteish and Needs [21] on GaSb have shown the necessity for including higher order terms to obtain a better description of strain splittings. We see that the  $n = 1$  superlattice levels are approximately the average of the strained germanium and silicon levels.

The states for the  $n = 1, 2, 3$  and  $n = 6$  superlattices are plotted in figure 3. We see that as  $n$  increases the valence band splitting increases and the lower  $\bar{X}$  state moves down. All these superlattices are indirect with a conduction band minimum along the  $\bar{\Delta}$  direction. The differences between the direct gaps and the indirect gaps are 0.99, 0.46, 0.71 and 0.71 eV for the  $n = 1, 2, 3$  and  $n = 6$  superlattices respectively. For the upper  $\bar{X}$  state there is a non-monotonic decrease in energy with  $n$ . The  $\bar{L}(111)$  states oscillate



**Figure 2.** Energy levels at symmetry points for silicon, the [111]  $\text{Si}_1/\text{Ge}_1$  superlattice, germanium strained to a (111) silicon substrate and unstrained germanium.



**Figure 3.** Energy levels at symmetry points for the  $n = 1, 2, 3$  and  $n = 6$  superlattices.

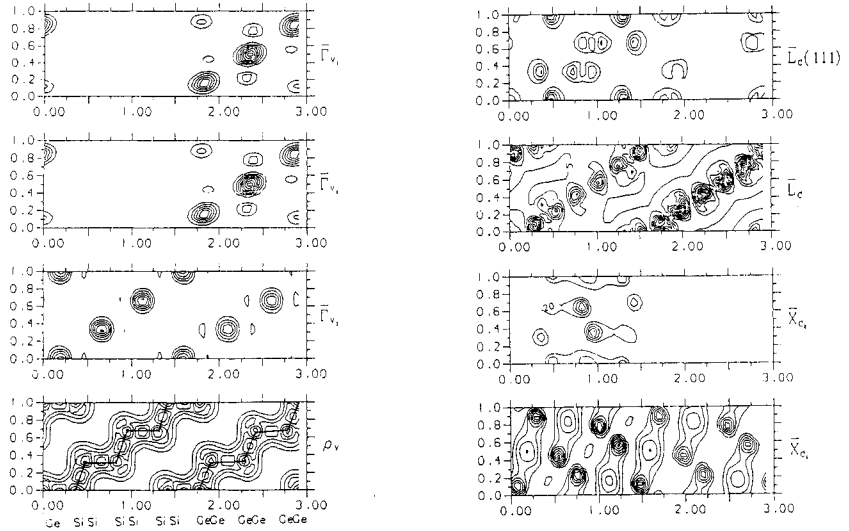
with  $n$ . For  $n = 1$  and  $n = 3$  the  $\bar{L}(111)$  state is at the  $A$  point and for  $n = 2$  and  $n = 6$  it is at the  $\Gamma$  point as mentioned above. The states folded onto the  $\Gamma$  point are much lower in energy. The remaining  $\bar{L}$  derived states mirror the behaviour of the  $\bar{L}(111)$  states. In interpreting the band structures from which figures 2 and 3 were compiled ‘true’ states were distinguished from ‘folded in’ states by a careful examination of charge density contours as mentioned above.

The  $n = 2, 3$  and  $n = 6$  superlattices all have a gap deep in the valence band although much smaller than that for the  $n = 1$  superlattice. This gap decreases non-monotonically as  $n$  increases. For  $n = 6$  the gap is only 0.12 eV. This valence band gap is found in the [001]  $\text{Si}_1/\text{Ge}_1$  superlattice [22] but not in the [001]  $\text{Si}_4/\text{Ge}_4$  superlattice [23] and illustrates a similarity between the [111] superlattices and the bulk  $\text{Si}_{0.5}\text{Ge}_{0.5}$  alloy which has a valence band gap.

### 3.2. Charge density contours

In figure 4 we plot the charge density contours at selected states for the  $n = 6$  superlattice. The plane chosen is that perpendicular to the interface containing a chain of bonds. The first plot in the figure is the total valence charge.

We see complete localization of charge on the germanium sublattice for the upper two valence band states. From figure 3 we note that as we go from  $n = 1$  to  $n = 6$ , the valence band splitting increases and probably will continue to increase for larger  $n$ . In the limit of large  $n$  the valence band splitting of the superlattice will be the same as the valence band splitting of strained germanium if the valence band offset for the interface



**Figure 4.** Charge density contour plots at selected states for the  $n = 6$  superlattice. The chain of bonds with labelling of the atoms is shown in the first plot.

is greater than the splitting of the strained germanium. The value we have calculated for the splitting of strained germanium using the planar spacings given in table 1 is 0.39 eV. This is the splitting shown in figure 2. The splitting of the  $n = 6$  superlattice is however calculated to be 0.64 eV contrary to our assertion. The reason for this is that the planar spacings for the strained germanium were calculated for the case of an infinite slab of strained germanium. When we repeated the calculation using the planar spacings taken from the germanium region of the  $n = 6$  supercell we get a splitting in the strained germanium of 0.78 eV. The calculated value of the valence band offset in this system is 0.75 eV [24] so the splitting of the strained germanium is greater than the valence band offset and in the limit of large  $n$  the superlattice valence band splitting should become of the same as valence band offset. A look at the band structure of the  $n = 6$  superlattice reveals that this will not in fact happen because the splitting is so large extra states from the [111] direction fold onto the  $\Gamma$  point in between the upper valence band states. Such a marked localization does not occur in [001] orientated Si/Ge superlattices with the same repeat distance [5, 6]. This difference in the degree of localization between the two orientations can be explained in terms of effective mass theory and the fact that the [111] heavy-hole mass for silicon is approximately twice that of [001] heavy-hole mass as can be seen from a plot of the silicon band structure.

All the lower conduction band states shown in figure 4 indicate a preferred localization of charge on the silicon sublattice indicating a type II superlattice offset.

#### 4. Summary

We have looked at the electronic structure and the charge density distribution of  $\text{Si}_n/\text{Ge}_n$  superlattices grown on a (111) silicon substrate for  $n = 1, 2, 3$  and  $n = 6$ . We find that none of these superlattices exhibit a direct gap. A notable feature of the  $n = 6$  superlattice is the complete localization of charge at the top of the valence band on the germanium sublattice.

It would seem probable that, if grown on a (111) germanium substrate, the  $n = 6$  superlattice may have a direct gap as the  $\bar{L}(111)$  point minimum of the germanium which folds exactly onto the  $\Gamma$  point will not be lifted by strain.

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