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Electronic structure of twinning superlattices

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Abstract

The electronic properties of a recently proposed new structure, twinning superlattice, based on the periodic array of twin boundaries in Si and Ge, are calculated. In addition to showing miniband structure as conventional superlattices do, the twinning superlattices exhibit some unusual electronic properties, such as zero energy gaps, interface state derived minibands, and indirect miniband gaps.

1. Introduction

It is well known that the periodicity in semiconductor superlattices gives rise to miniband-like electronic structure. This is usually perceived to be caused by the periodically varying conduction and valence band edges which in turn have their roots in variation of either the material composition or electrostatic potential. Alternatively, the miniband formation can also be viewed as a consequence of the coherent electron scattering at the periodically distributed interfaces. An important point to realize is that it is the very existence of the periodic scattering, rather than the underlying mechanism, which generates minibands. However, a spatially varying potential is not the only way to introduce electron scattering in low-dimensional semiconductors. The possibility also exists to make a single semiconductor material behave as an inhomogeneous structure. This can be done in at least two ways, resulting in nontraditional concepts of the superlattice structure: one relying on crystal polytypism, and another on variable orientation.

Polytypic (or heterocrystalline) superlattices would rely on the possibility of coexistence of fcc and hcp crystalline forms in some semiconductors, due to the small difference in their energies (SiC and ZnS being typical examples) [1,2]. It is possible to conceive polytype superlattices as a periodic repetition of a specific polytypic sequence of the constituent semiconductor. Although the two crystal phases are different, they are essentially perfectly lattice-matched at the interface, and all the bonds are preserved.

Another method of introducing periodic "scattering centers" in a semiconductor is to make the crystal orientation variable, in such a way that no dangling bonds appear at the interface of the two differently oriented semiconductors. Single defects of this type are known as stacking faults, most commonly observed in crystalline semiconductors with diamond and zincblende structures as well as in many metals. The most elementary stacking fault is the twin stacking fault (or twin

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boundary). It comprises the reversal of the stacking sequence along [111] at some plane, i.e. instead of the AA'BB'CC'AA'BB'CC' sequence of the perfect crystal one now has AA'BB'CC'A | A' CC'BB'AA', where AA' (or BB', CC') denotes the two basis atoms of the primitive unit cell. Formally, a twin stacking fault can be constructed by cutting the [111] directed bonds in (say) the AA' layer, rotating half of the crystal by 180° about the bond axis, and then reconnecting all cut bonds of the two crystal halves.

We have recently proposed a new type of superlattice [3], based upon periodic reversal of the atomic stacking sequence, i.e. periodically distributed twin boundaries, in a semiconductor. One period of an (m, n) twinning superlattice would include n and m atomic bilayers of oppositely oriented material. While the interface between the two crystal orientations is perfectly lattice-matched, the wavefunctions are symmetry-mismatched. This symmetry mismatch gives rise to rather large electron scattering at the interface, which has indeed been observed in single stacking faults, especially for energies close to the band edge [4,5]. Twinning may be found in a large number of minerals [6]. In this paper, however, we have studied Si and Ge based twinning superlattices.

Recently, homoepitaxial MBE growth of a single twin boundary in Si has been successfully achieved with the help of boron submonolayer induced surface reconstruction. This method might, in our opinion, be extended towards growing twinning superlattices (the role of boron is only temporary, and once the twin boundary is made, it can be removed and/or compensated by some other dopant [7]). Another approach, at least for some classes of twinning superlattices, might include the application of indentation technique [8].

2. Theoretical details

We have calculated the miniband structure of the twinning superlattices using the layer method [9,10], based upon empirical pseudopotentials utilising the standard form factors for Si [11] and Ge [12]. The method is numerically very stable and allows the direct interpretation of the results in terms of the bulk band structure of the constituent materials.

We have concentrated upon the conduction band properties. Here the two materials differ both in the ordering of Γ, X and L valleys and the relative spacing (~ 1 eV in Si and ~ 0.2 eV in Ge) so that band mixing, for example, is expected to be more prominent in Ge than in Si based superlattices.

On formation of the superlattices the new interface Brillouin zone is such that the mapping of the principal valleys is onto the $\bar{M}$ and $\bar{\Gamma}$ points. The results presented here are, therefore, for the $\bar{M}$ and $\bar{\Gamma}$ points though we have explored the whole of the irreducible zone.

3. Results for Si based twinning superlattices

The miniband electronic structure of Si based $(n, 1)$ and (n, n) twinning superlattices, at the interface Brillouin zone point close to $\bar{M}$, corresponding to the local (and global) X valley minimum, is displayed in Fig. 1. For the $(n, 1)$ superlattices the positions of miniband edges in the superlattice Brillouin zone, vary with the superlattice structure, and are always off the Brillouin zone center or edges (Fig. 2). Also displayed in Fig. 1 is the composition of various superlattice states in terms of the contribution of various bulk states to the full wavefunction squared. The figures show that the bulk X_3 and L states, though remote and thus very evanescent, are rather highly excited, due to the symmetry mismatch at the interface.

The (n, n) superlattices have a symmetric miniband dispersion, with the lowest point at the superlattice Brillouin zone center, as shown in Fig. 2. A distinct feature of (n, n) superlattices is the occurrence of zero energy gaps at the superlattice Brillouin zone boundary. Zero energy gaps actually occur not only at $\bar{M}$ but in fact at any point of the interface Brillouin zone. This is a manifestation of the screw symmetry characterizing the unit cell (period) of this type of superlattice [13].

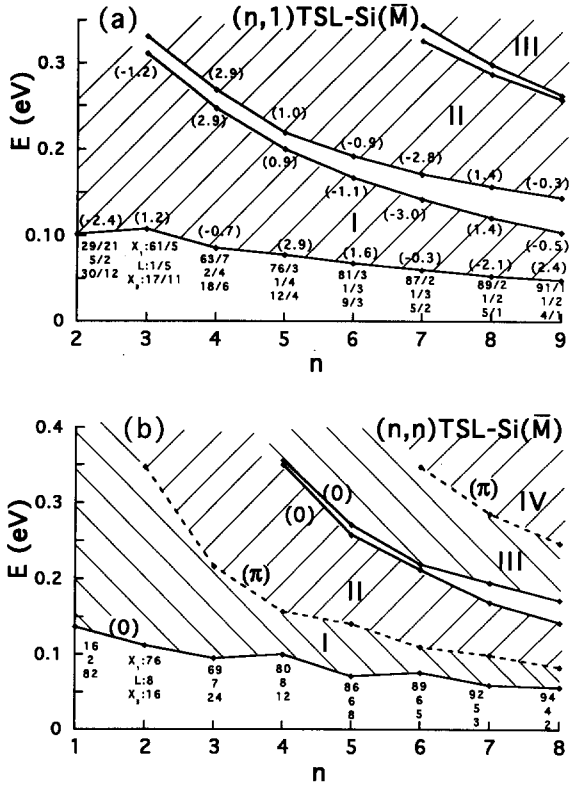

Fig. 1. Allowed minibands in (a) Si based $(n, 1)$ and (b) Si based (n, n) twinning superlattices, close to the $\bar{M}$ point (the bulk X valley bottom, from which the energy is measured). Solid lines connect miniband edges and broken lines indicate the zero energy gap points. Points of miniband extrema in the superlattice Brillouin zone (in units such that $-\pi \leq k_{SL}d \leq \pi$) are given in brackets. Composition of the superlattice state at the lowest miniband bottom is also given. (The notation is the following. In the case of $(n, 1)$ superlattice X_1:z1/z2, L: z3/z4,... means that out of the total wavefunction squared in a superlattice period, z1 percent is the bulk X_1 state contribution in the first layer with n atomic bilayers and z2 percent in the second layer with one atomic bilayer. In the case of (n, n) superlattice, the wavefunction is evenly distributed among the two half-periods, and only the overall contributions of bulk states are given.)

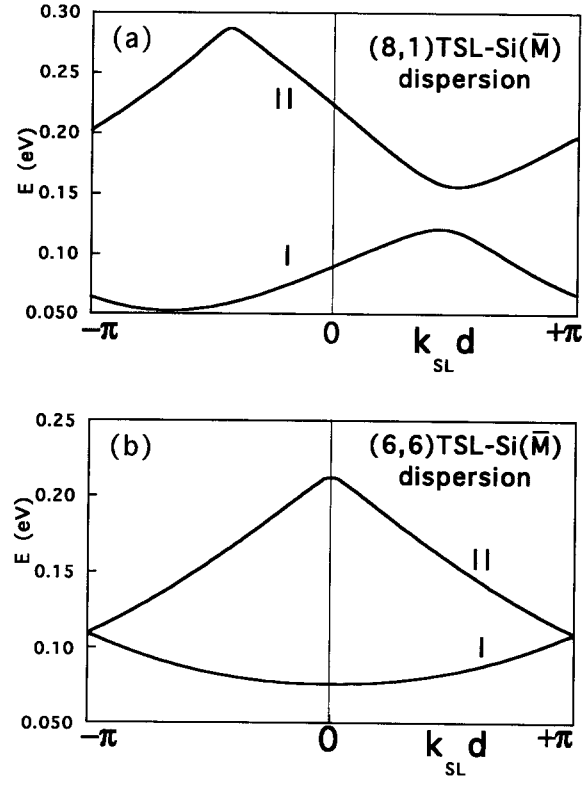

Fig. 2. Dispersion of the lowest two minibands in (a) Si based (8,1) and (b) Si based (6,6) superlattices at the $\bar{M}$ point of the interface Brillouin zone (k_{SL} is the superlattice wavevector).

The calculated electronic structure of (n, n) Si based twinning superlattice at the $\bar{\Gamma}$ point of the interface Brillouin zone is given in Fig. 3. In this case the lowest pair of minibands is derived from an interface bound state. As the superlattice period increases, the width of these minibands decreases towards the single twin stacking fault bound state from which they originate. Arising

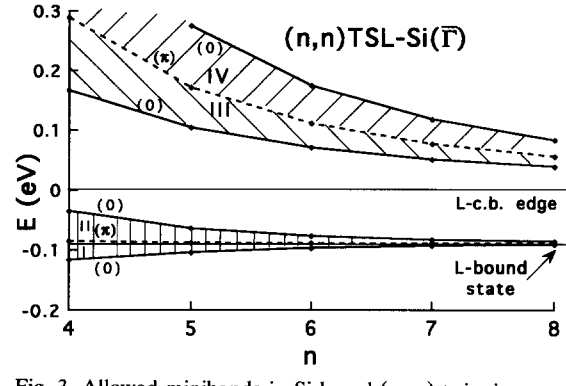

Fig. 3. Allowed minibands in Si based (n, n) twinning superlattices at the $\bar{\Gamma}$ point of the interface Brillouin zone (the bulk L valley bottom, from which the energy is measured). Solid lines connect miniband edges and broken lines indicate the zero energy gap points. Whether evanescent or propagating, only the bulk L states contribute to the superlattice state.

from interface states, these exhibit almost purely L character (Γ–L mixing is very low). The miniband wavefunctions are composed of pairs of growing and decaying evanescent L states. The energy range spanned by these minibands is at least partly (fully for longer periods, $n \geq 6$) below the lowest conduction band edge (i.e. the L valley). This is, to our knowledge, the only example of a superlattice with some of its minibands formed entirely from the evanescent bulk states.

4. Results for Ge based superlattices

Calculations of the electronic structure of Ge based twinning superlattices show that while they share some common features with Si based ones, they also display remarkable differences. The valleys L, X_1 and X_3 are much closer to each other in Ge than in Si, and thus strongly interact, and thus quantitative differences in the results at $\bar{M}$ are expected. This is illustrated in Fig. 4 which shows the miniband dispersion for the (6,6) superlattice at $\bar{M}$. The dispersion is clearly anomalous with local extrema inside the Brillouin zone. This occurs in the even index minibands for (even,even) superlattices and the odd index ones for the (odd,odd) case. This effect gradually diminishes at higher energies.

Analysis of the eigenstates corresponding to these bands shows that the states, although evanescent, are highly excited and not only contribute a larger part of the overall charge density than the propagating L state but also carry a considerable fraction of the total current. The extrema of the anomalous minibands are characterized by two large X and L state current counterflows, which cancel at the exact extremum point.

The miniband dispersion in the Ge based (5,6) superlattice is also given in Fig. 4. In this case the dispersion is much more structured due to the X–L interaction, and has *indirect miniband gaps,* unlike any other type of superlattice.

At the $\bar{\Gamma}$ point, where Γ–L mixing is not large, there is great similarity between Si and Ge based superlattices. The only real difference is that in Si the minibands at $\bar{\Gamma}$ are well above those at $\bar{M}$ in

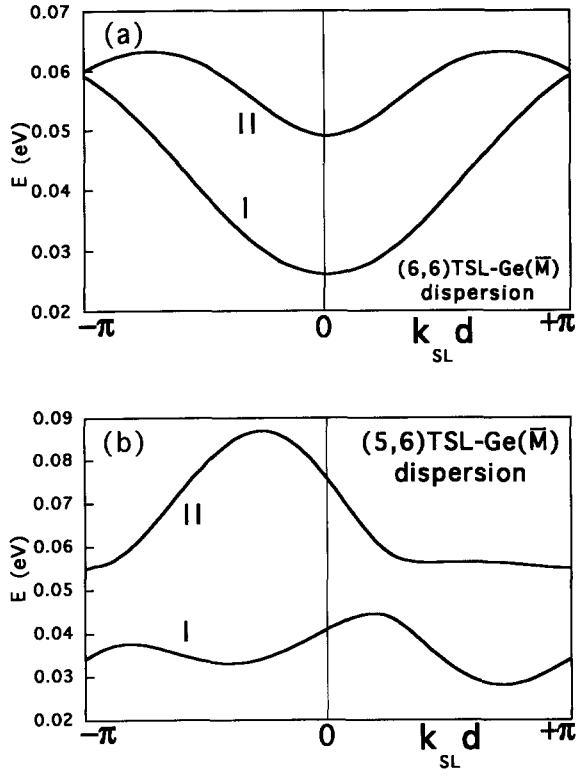

Fig. 4. Dispersion of the lowest two minibands in (a) Ge based (6,6) and (b) Ge based (5,6) twinning superlattices at the $\bar{M}$ point of the interface Brillouin zone.

energy, while in Ge these are closely located, since its lowest valley (L) projects onto both the $\bar{\Gamma}$ and $\bar{M}$ points.

5. Summary

We have presented calculations of electronic miniband structure for twinning superlattices based on Si and Ge. Both Si based as well as Ge based (n, n) superlattices are found to be characterized by zero energy gaps across the interface Brillouin zone. In general the energies and widths of the minibands in the twinning superlattices are such that they would enable (for n-doped materials) inter-miniband absorption spectrum in the infrared. In addition, in spite of the fact that the constituent bulk semiconductor is an indirect band gap material, interband transitions are pos-

sible from valence to conduction band in twinning superlattices because the folded conduction band is direct, though the eigenstate composition would suggest weak oscillator strengths. The (m, n), $m \neq n$, superlattices show more structured miniband dispersion, with indirect band gaps.

Our results thus show that twinning superlattices would offer much versatility in tailoring the electronic miniband structure. Certainly the two principles of building superlattice periodicity (crystal orientation and material composition/doping) may be combined to extend the possibilities of "band structure engineering" even more, once the means of fabricating twinning superlattices are devised. Such fabrication may be expected quite soon in view of the recent advances in fabricating high quality single twin boundary [7], the building block of twinning superlattices. These systems offer the significant benefits of simple chemistry, lack of stress and a favoured technological environment.

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7. References

[1] C.-Y. Yeh, Z.W. Lu, S. Froyen and A. Zunger, Phys. Rev. B 46 (1992) 10086.
[2] A. Qteish, V. Heine and R.J. Needs, Phys. Rev. B 45 (1992) 6534.
[3] Z. Ikonić, G.P. Srivastava and J.C. Inkson, Solid State Commun. 86 (1993) 799.
[4] M.D. Stiles and D.R. Hamann, Phys. Rev. B 38 (1988) 2021.
[5] M.D. Stiles and D.R. Hamann, Phys. Rev. B 41 (1990) 5280.
[6] C.A. Sorrel and G.F. Sandstrom, The Rocks and Minerals of the World (Collins, London, 1977).
[7] R.L. Headrick, B.W. Weir, J. Bevk, B.S. Freer, D.J. Eagelesham and L.C. Feldman, Phys. Rev. Lett. 65 (1990) 1128.
[8] P. Pirouz, R. Chaim, U. Dahmen and K.H. Westmacott, Acta Metall. 38 (1990) 313.
[9] D.Y.K. Ko and J.C. Inkson, Phys. Rev. B 38 (1988) 9945.
[10] Z. Ikonić, G.P. Srivastava and J.C. Inkson, Phys. Rev. B 46 (1992) 15150.
[11] J.R. Chelikowsky and M.L. Cohen, Phys. Rev. B 14 (1976) 556.
[12] M.L. Cohen and T.K. Bergstresser, Phys. Rev. 141 (1966) 789.
[13] S.L. Altmann, Band Theory of Solids: An Introduction from the Point of View of Symmetry (Clarendon, Oxford, 1991).