Electronic band structure and nonparabolicity in strained-layer Si-$Si_{1-x}Ge_x$ superlattices

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We report a pseudopotential calculation of the nonparabolicity of the conduction and valence minibands for Si-$Si_{1-x}Ge_x$ strained-layer superlattices of period 10–30 Å. We find that the conduction-band nonparabolicity in directions both perpendicular (z) and parallel to the interface planes is several orders of magnitude larger than that for bulk silicon and is comparable in magnitude with the value for bulk GaAs. Along the superlattice axis (z), the conduction-band nonparabolicity is dominated by virtual transitions involving the lowest conduction states and strongly reflects the energy separation between them. Since this separation depends on strain and layer widths, the magnitude of this nonparabolicity can be "tuned" over 2 orders of magnitude. In the valence band, and along the direction parallel to the interface planes in the conduction band, the nonparabolicity is dominated by virtual excitations across the fundamental gap. The effective masses are also presented. A comparison is given of the mechanisms determining band nonparabolicity in Si-$Si_{1-x}Ge_x$, GaAs-$Ga_{1-x}Al_xAs$, and GaAs-$GaAs_{1-x}P_x$ superlattices.

I. INTRODUCTION

Recent calculations by Morrison *et al.*[1] using a pseudopotential scheme have revealed several interesting features of Si-$Si_{1-x}Ge_x$ strained-layer superlattices. The effect of strain in Si-$Si_{0.5}Ge_{0.5}$ (001) superlattices grown on a buffer layer of $Si_{0.75}Ge_{0.25}$ causes the conduction electrons to be confined in the silicon layers [Fig. 1(a)]. This is the result predicted by the pseudopotential method,[2] in agreement with the experimental findings of Abstreiter *et al.*[3] However, if the atoms are assumed to occupy the cubic positions of a conventional unstrained superlattice, then the electrons are confined in the alloy layers [Fig. 1(b)]. Therefore, in these structures the strain not only affects the degree of confinement, but determines the layer in which the electrons are confined. Quantitative results have also been obtained which demonstrate the enhanced momentum mixing, brought about by the combined effects of strain and zone folding. The most important result is the effect on the optical matrix elements across the superlattice band gap. In systems with ultrashort periods the oscillator strength of this transition is enhanced to within 2 orders of magnitude of that associated with direct-gap materials (Fig. 2).

The results presented so far are concerned with the basic features of the electronic structure of the Si-$Si_{1-x}Ge_x$ strained-layer superlattice, e.g., band gaps and principal transitions. In this paper we report calculations of higher-order effects in these systems that give a better understanding of the details of the electronic band structure. In particular, we concentrate on the virtual-excitation processes which determine the band curvature at important k points and compute effective masses and band nonparabolicities. No such results are available in the literature.

Dispersion curves are presented showing the variation in energy through the Brillouin zone for the states near the band edges. Nonparabolicities are determined in directions both parallel and perpendicular to the interface planes for the conduction- and valence-band–edge states.

We have focused most of our attention on the superlattice conduction band. It turns out that in this case the

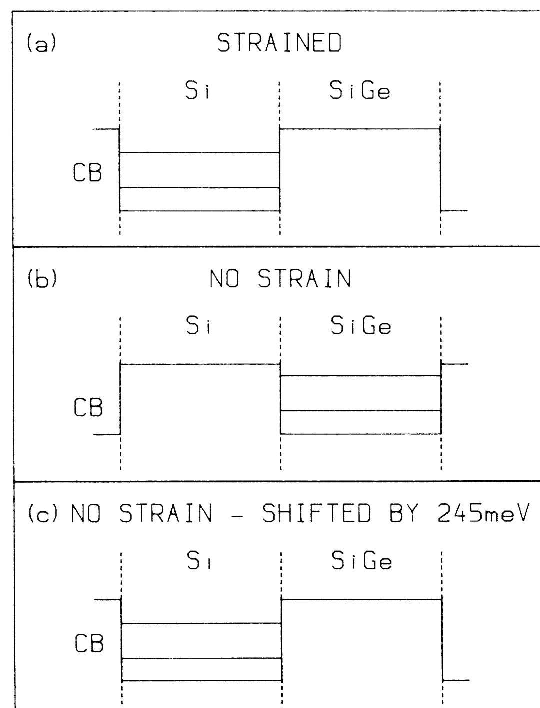

FIG. 1. Sketch of the confined electron states in the conduction band for (a) the strained model, (b) the "unstrained" model, and (c) the "unstrained" model with the pseudopotentials shifted by 245 meV.

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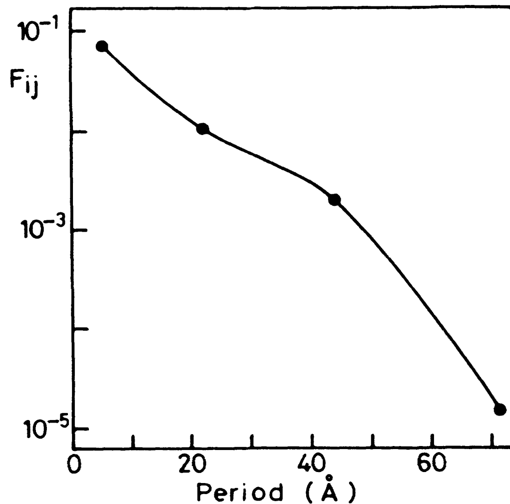

FIG. 2. Plot of the oscillator strength, associated with the transition across the fundamental gap, as a function of the superlattice period.

band curvature is of quite different origin compared to that reported for other materials, for example, GaAs-$Ga_{1-x}Al_xAs$ (Ref. 4) and GaAs-$GaAs_{1-x}P_x$ (Ref. 5). The conduction minima in bulk silicon lie along the Δ line in the Brillouin zone towards the zone-edge X points. Consequently, the zone folding along the superlattice [001] axis causes the position of the folded minimum within the superlattice Brillouin zone to vary as a function of the superlattice period. Also, the superlattice states with energies lower than that of the bulk X point are found to be quasidegenerate. The band structure in the region of the bulk minima is nearly-free-electron-like, and therefore the bands are virtually parabolic. In the superlattice the enhanced momentum mixing causes new transitions to be allowed which greatly affect the curvature of the band. The most significant virtual transition in the short-period superlattices discussed here is that between the quasidegenerate ground states, which are both related to the bulk minimum. In contrast, the minima of the GaAs-$Ga_{1-x}Al_xAs$ (Ref. 4) and GaAs-$GaAs_{1-x}P_x$ (Ref. 5) superlattices are at the Brillouin-zone center, Γ, and the principal virtual excitations are between either the valence states or the conduction states from the folded bulk X point.

A further difference occurs in the directions parallel to the interface planes. In the GaAs-based superlattices the conduction-band curvature in these directions is unchanged from that of bulk GaAs. In bulk silicon there are six equivalent conduction minima in the [100], $[\bar{1}00]$, [010], $[0\bar{1}0]$ [001], and $[00\bar{1}]$ directions. As a result of this symmetry in the energy surfaces the nonparabolicity is the same in the [100], [010], and [001] directions. In the Si-$Si_{1-x}Ge_x$ superlattice, the effect of strain is to split the minima into a fourfold- and a twofold-degenerate state. In the systems considered here the conduction electrons are confined in the silicon layers, and the twofold-degenerate minima in the silicon is lower in energy than the fourfold-degenerate state. Therefore the conduction electrons will principally be found in the twofold-degenerate minima, which are aligned with their major axis parallel to the superlattice axis. Thus the nonparabolicity which affects the transport of electrons in the direction parallel to the interface planes is determined by the curvature of the twofold-degenerate minima in the direction of the transverse mass.

Our results show that the conduction-band nonparabolicity in directions both perpendicular and parallel to the interface planes is increased relative to that in bulk silicon, and is comparable to that in bulk GaAs.

In the bulk valence band the maximum is at Γ, and so the position of the band extremum (maximum) is unaffected by the zone folding. The uppermost valence states are confined in the alloy layers, and the valence band in the bulk alloy is distinctly nonparabolic. We find that the nonparabolicity in the superlattice is of the same order of magnitude as that in the bulk material.

Effective masses for the conduction and valence bands are also presented. The conduction-band values are only given for the twofold minima since the effective masses in the fourfold minima are bulklike.[1] The zone folding is expected to affect the longitudinal masses, while the strain can affect both the longitudinal and transverse masses. We find that only the conduction-band longitudinal effective mass is significantly different than the bulk value.

II. METHOD OF CALCULATION

The procedure used for these calculations is based on the pseudopotential approach of Jaros *et al.*[6,7] The application of this method to Si-$Si_{1-x}Ge_x$ strained-layer superlattices is described in detail in Ref. 1. In all the systems considered here it is assumed that the superlattice is grown on a buffer layer of $Si_{1-y}Ge_y$, where the layer of y corresponds to the overall germanium concentration of the superlattice. In this arrangement the strain is distributed symmetrically in both constituent layers. The lattice constant parallel to the interfaces is taken to be that of the buffer layer, while the perpendicular lattice constants in each material are calculated by minimizing the elastic strain energy.[8,9] The superlattice wave functions ψ are obtained as an expansion of the buffer-layer eigenfunctions ϕ_{nk},

$$\psi=\sum_{n,k} A_{nk}\phi_{nk} , \tag{1}$$

where n is the band index and k the wave vector.

Except where stated otherwise, the systems described in these calculations are Si-$Si_{0.5}Ge_{0.5}$ superlattices. It is assumed that the unit cell contains equal numbers of silicon and alloy atoms, and therefore the buffer layer is $Si_{0.75}Ge_{0.25}$.

The maximum-period superlattice considered here is 27.5 Å, the reason for this limitation being as follows. The superlattice wave functions in Eq. (1) are formed from an expansion of the bulk eigenfunctions in the buffer layer. For these calculations the expansion set was limited to the three uppermost valence bands and the

four lowest conduction bands. Morrison *et al.*[1] have demonstrated that this is sufficient for calculations with periods of up to 44 Å.

The nonparabolicity of a system determines the extent to which the band structure at an extremum deviates from the parabolic form, where the energy E is proportional to the square of the wave vector k. In symmetric structures a dependence of E on odd powers of k is ruled out by symmetry. Consequently, the lowest-order correction to the parabolic relation is given by a term which depends on k to the fourth power, i.e., the energy can be written as

$$E = Ak^2 + Bk^4 + \cdots . \tag{2}$$

Thus the magnitude of the nonparabolicity is given by the fourth derivative of the band energy E, with respect to the wave vector k. Energy-versus-wave-vector dispersion curves are shown in Figs. 3–5. However, a calculation of the fourth derivative by a visual inspection of the curves is impractical and likely to lead to considerable error.

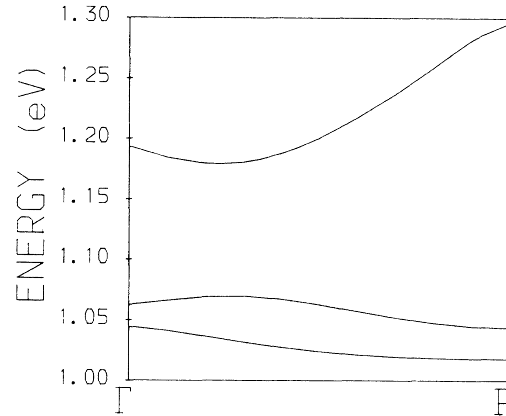

FIG. 4. Conduction-band dispersion relations for a 22.0-Å-period Si-$Si_{0.5}Ge_{0.5}$ strained-layer superlattice.

Instead, the value of d^4E/dk^4 is calculated as follows. Using perturbation theory the fourth order approximation to the energy in the superlattice band N, for which the fourth derivative is required, can be written as

$$E_N^{(4)} = \sum_{s\neq N}\sum_{t\neq N}\sum_{u\neq N} \frac{V_{sN}V_{ts}V_{ut}V_{Nu}}{E_{sN}E_{tN}E_{uN}} - \sum_{t\neq N}\sum_{u\neq N} \frac{V_{tN}V_{NN}V_{ut}V_{Nu}}{E_{tN}^2 E_{uN}} - \sum_{s\neq N}\sum_{u\neq N} \frac{V_{sN}V_{us}V_{NN}V_{Nu}}{E_{uN}^2 E_{sN}} + \sum_{u\neq N} \frac{V_{NN}^2 \mid V_{uN}\mid^2}{E_{uN}^3} - \sum_{s\neq N}\sum_{u\neq N} \frac{\mid V_{sN}\mid^2 \mid V_{uN}\mid^2}{E_{uN}^2 E_{sN}} , \tag{3}$$

where $E_{ab} = E_a - E_b$, and s, t, and u label the superlattice states. The potential terms V are given by a $\mathbf{k}\cdot\mathbf{p}$ expansion due to Kane,[10]

$$V_{nn'} = (\hbar^2/m)(k^2 - k_0^2)\delta_{nn'} + (\hbar/m)(\mathbf{k} - \mathbf{k}_0)\cdot\mathbf{M}_{nn'}(\mathbf{k}_0) . \tag{4}$$

$\mathbf{k}_0$ is the wave vector at which the superlattice calculation is performed, and the matrix elements are

$$\mathbf{M}_{nn'}(\mathbf{k}_0) = \int u_{n'}^*(\mathbf{k}_0, \mathbf{r})\mathbf{p}u_n(\mathbf{k}_0, \mathbf{r})d\mathbf{r} , \tag{5}$$

$\mathbf{p}$ being the momentum operator. By differentiating Eq. (3) four times with respect to k and substituting for the matrix elements $\mathbf{M}_{nn'}(\mathbf{k}_0)$ and the eigenvalues at the wave vector k, the value of d^4E/dK^4 can be found.

Thus the value of d^4E/dK^4 is given by the product of four matrix elements divided by the product of three energies, the energies being measured from the band for which the nonparabolicity is required. The states nearest in energy to the relevant band, and between which transitions are allowed, most affect the nonparabolicity of that band.

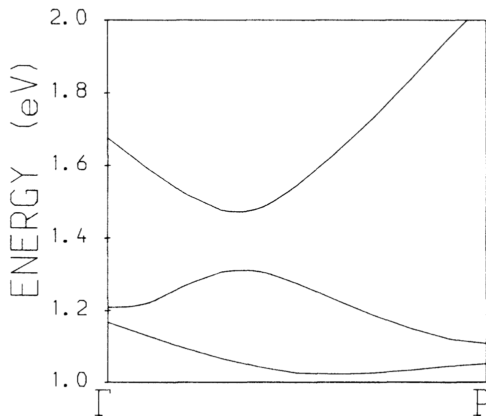

FIG. 3. Energy-vs-wave-vector dispersion relations for the three lowermost conduction bands of an 11.0-Å-period Si-$Si_{0.5}Ge_{0.5}$ strained superlattice. The dispersion is shown along the superlattice axis from the Brillouin-zone center, Γ to the superlattice Brillouin-zone edge P. The energies are measured from the top of the valence band at Γ.

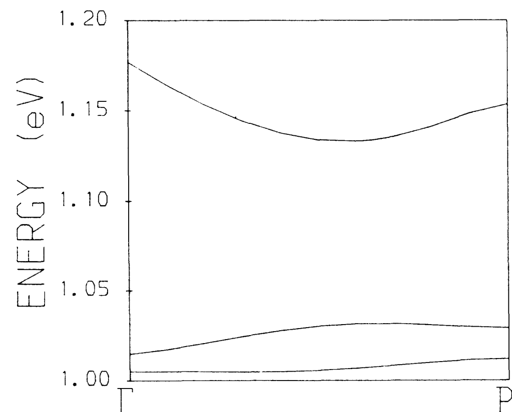

FIG. 5. Conduction-band dispersion relations for a 27.5-Å-period Si-$Si_{0.5}Ge_{0.5}$ strained-layer superlattice.

A much simpler approach can be used initially to determine qualitatively the factors which affect the nonparabolicity. Consider that E_a is the parabolic approximation to the eigenvalue equation, where

$$E_a = \frac{\hbar^2 k_a^2}{2m} . \tag{6}$$

Then, in the nondegenerate case it can be shown (e.g., see p. 12 of Ref. 11) that the second-order correction to this is to include the effects from other states so that

$$E(k) = E_a + \sum_{k'} \frac{|V_{k'}|^2}{E_a - E'} , \tag{7}$$

where the $V_{k'}$ represent the Fourier components of the periodic potential. Therefore states which are lower in energy than E_a will tend to raise the energy $E(k)$, while states which are higher in energy will tend to lower $E(k)$. If the dominant transitions are from the lower-energy states, then the band in question will bee raised in energy above the parabolic approximation, and therefore the value of B in Eq. (2) will be positive. Conversely, if the higher states dominate in the transitions, then the band will be pushed below the parabolic form, and so the value of B will be negative.

Nonparabolicities for two other systems, an "unstrained" Si-$Si_{1-x}Ge_x$ superlattice and a bulklike structure, have also been evaluated for comparison with the strained superlattice results. Both systems can be modeled using this pseudopotential scheme of the strained superlattice but with minor changes.

The "unstrained" Si-$Si_{1-x}Ge_x$ superlattice has been studied previously by Morrison *et al.*[2] The atoms are placed in a cubic arrangement with the lattice constant throughout the superlattice being that of the substrate. This represents an unstrained system in the fact that the atoms occupy cubic lattice positions rather than being displaced to form tetragonal unit cells as in the strained model. The unstrained model does not represent a real superlattice, i.e., one that could be constructed, but is useful in determining how the strain, as manifested in the displacement of the atoms, affects the band structure. The strain also affects the barrier potential,[12] and for Si-$Si_{0.5}Ge_{0.5}$ the change is such that electrons in the unstrained model are confined in the alloy [Fig. 1(b)].[2] Consequently, a calculation of the conduction-band nonparabolicity in the unstrained system described above would result in a value of the band nonparabolicity in the alloy. Since the electrons in the strained system are confined in the silicon layers, this would not be a useful comparison. The situation can be rectified by rigidly shifting the conduction bands of the alloy and the silicon relative to each other so as to obtain confinement in the silicon layers. For these calculations a shift of 245 meV is applied [Fig. 1(c)].

In the bulklike calculation the atoms are assumed to occupy cubic lattice positions, as in the unstrained superlattice, but the superlattice is filled with either silicon atoms or alloy atoms.

III. NUMERICAL RESULTS

In this section we examine the various features of the band curvatures and the mechanisms responsible for these effects. The dispersion and nonparabolicity are discussed in three subsections. In the conduction band the effects observed along the superlattice axis are treated separately from those seen in the directions parallel to the interfaces since the important virtual transitions are very different in the two cases. In the valence band the nonparabolicities in both directions are discussed together. The effective masses in both bands are discussed in a fourth subsection. Comparison with a bulklike calculation has been included where possible.

A. Conduction-band nonparabolicity along the superlattice axis

The results described in this subsection relate to Si-$Si_{0.5}Ge_{0.5}$ superlattices where the unit cells contain equal numbers of silicon and alloy atoms. The buffer layer is therefore $Si_{0.75}Ge_{0.25}$.

In the "unstrained" superlattice calculations the silicon and alloy conduction bands are adjusted relative to one another by 245 meV as described in Sec. II. This ensures that the electron confinement in the conduction band is roughly the same in both the strained and unstrained models. The shift also affects the valence band, but the valence-band potential barrier is large, so any adverse effects should be limited. Also, the results show that the band curvature in this direction is virtually unaffected by transitions from the valence band; therefore any changes in the valence-band energy levels should have a negligible effect.

For the bulk calculations the superlattice is filled with silicon atoms, this being a relevant comparison since in the superlattice the electrons are confined in the silicon layers.

The energy–versus–wave-vector dispersion curves along the superlattice axis are presented in Figs. 3–5 for periods between 11.0 and 27.5 Å. The curves are generated using a $\mathbf{k}\cdot\mathbf{p}$ expansion about a superlattice calculation at a single k point, except in the 11.0-Å-period case, where, due to the size of the superlattice Brillouin zone, the curve is constructed from $\mathbf{k}\cdot\mathbf{p}$ calculations about two k points in the zone. The validity of the $\mathbf{k}\cdot\mathbf{p}$ method can be seen by comparing the curves for the two lowest conduction bands in Figs. 4 and 5 with those published by Morrison and Jaros,[13] which are the result of a series of superlattice calculations at various values of k in the range of $\Gamma - P$.

The calculated values of d^4E/dk^4 at the Brillouin-zone center Γ and at the folded minimum along the superlattice axis are given in Table I. In comparison, the bulk silicon calculation yields a value of less than $+10^{-4}$ eV Å^4. In fact, the superlattice results are comparable in magnitude with the value of d^4E/dk^4 in bulk GaAs of 3.8×10^4 eV Å^4 obtained by Brown *et al.*[4] Three main points can be noticed from these results. First, all of the superlattice systems considered here have significantly nonparabolic conduction bands. Second, the results obtained with the unstrained model are within a factor of 2

TABLE I. The values of d^4E/dk^4 for the ground-state conduction band in the direction perpendicular to the interfaces. The results, in units of eV Å^4, are given at the ground-state conduction-band minimum and at Γ for both strained and unstrained lattices. The corresponding value for bulk GaAs is 3.8×10^4 eV Å^4.

		Strained	Unstrained
11.0-Å period	minimum	-1.9×10^3	-1.8×10^3
22.0-Å period	minimum	-6.0×10^3	-5.2×10^3
	Γ	-6.6×10^5	-1.0×10^6
27.5-Å period	minimum	-2.4×10^4	-2.3×10^4
	Γ	-3.7×10^5	-6.2×10^5

of those from the strained model. Third, the values of d^4E/dk^4 vary by 2 orders of magnitude. These points are discussed below.

The results in Table I indicate that the superlattice conduction band is distinctly nonparabolic. By comparison, the conduction band in bulk silicon is very nearly parabolic for a large range of values of k around the bulk minimum. In fact, the value of d^4E/dk^4 in the superlattice is enhanced by a factor of at least 10^7 relative to the bulk. The sign of the fourth derivative is also altered since in the superlattice calculations the result is negative, while in the bulk case it is positive. To understand the reasons for these differences it is necessary to consider which virtual excitations are responsible for the nonparabolicity in the two cases.

Consider the bulk system first. The nearest states in energy to the ground-state conduction band and, therefore, from the discussion in Sec. II, the states which are most likely to affect the nonparabolicity, are the adjacent conduction states. In bulk silicon the transitions between these states are disallowed, so the related matrix elements are virtually zero. Finite matrix elements are obtained in transitions between the conduction ground state and the valence band, but these transitions are weak and the energy separation is relatively large (greater than 1 eV); therefore, the band remains very nearly parabolic. The principal transitions are from states which are lower in energy, and the value of d^4E/dk^4 is positive, showing that the band has been pushed in energy as predicted by Eq. (7).

In the strained superlattice, recent results[13] have shown that the matrix elements across the band gap are enhanced by up to 3 orders of magnitude in comparison with the "unstrained" model. Therefore, an increase in the value of d^4E/dk^4 is expected for the strained system which should not be seen in the calculations with the "unstrained" model. However, the contribution to the fourth derivative from these interband transitions is negligible in comparison to that from intraband excitations between the lower conduction states. In particular, the virtual transition between the two lowermost conduction states is the most significant in terms of the effect of the ground-state nonparabolicity. The existence of a finite transition probability between these two states is quite remarkable since they are quasidegenerate, both originating from the bulk minimum. The contribution of these virtual excitations is enhanced by the quasidegeneracy, i.e., the splitting between the states is small. Since the transitions which make the conduction band nonparabolic are from states which are higher in energy, the effect is to push the ground-state energy below the bulk (parabolic) band and, therefore, the value of d^4E/dk^4 is negative.

The similarity between the results with the strained and unstrained models is at first sight unexpected because the optical matrix elements across the superlattice band gap are known to be enhanced by several orders of magnitude. The results are seen to differ by factors of up to 2, but this is a comparatively small effect in comparison with the variation from the bulk-silicon nonparabolicity. It is important, however, to realize that the similarity between the two results does not mean that the strain has little effect on the nonparabolicity. It has already been shown that in the absence of strain the electrons are confined in the alloy rather than in the silicon layers. This effect of the strain on the microscopic potential has been accounted for by rigidly shifting the conduction bands, as described in Sec. II. Thus the similarity of the strained and unstrained results actually shows that for the purpose of calculating conduction-band nonparabolicities the effect of strain can be estimated by simply adjusting the potential barriers to reflect the strained superlattice confinement. This makes it possible to model similar structures in a much simpler way, i.e., without recourse to the full-scale strained-layer calculation.

It has been stated above that the enhancement in the matrix element across the gap in the strained model has little effect on the conduction-band nonparabolicity. However, it is necessary to explain why the matrix element between conduction states should be virtually the same in both the strained and unstrained models, while the matrix element across the band gap varies by several orders of magnitude. The reason for this difference can be explained as follows. The optical matrix element describes the transition probability between the valence-band maximum at Γ and the conduction-band minimum near X. The enhancement of this matrix element due to strain demonstrates a mixing across the entire Brillouin zone and, therefore, over a short range in real space. By contrast, the lowermost conduction states, which determine the fourth derivative, are all localized in the same small region of k space. Therefore the mixing which enhances these matrix elements is of short range in k space and of long range in real space. The small deviations in the atomic positions due to strain give a short-range effect in real space, which enhances the mixing over a large region of k space, while the superlattice potential acts over a relatively long range in real space and, therefore, over only a localized region of k space.

The range of values of d^4E/dk^4 in Table I covers 2 orders of magnitude, although the period only varies by a factor of 2.5. There is some correlation between the magnitude of the fourth derivative and the energy separation of the lowest two conduction states. As the energies of the two states come closer together, the fourth derivative increases. There are, of course, other factors involved

since, as the energies change, so the transition probabilities between the states change, and the contributions from higher states cannot be neglected. A twofold reduction in the energy separation of the first two states does not necessarily increase the fourth derivative by a factor of 2^3; however, the results do suggest that the magnitude of the fourth derivative could be significantly enhanced by suitably tuning the properties of the lowermost conduction states. Such tuning can readily be achieved by changing the layer widths, or by altering the alloy concentration of either the constituent layers or the substrate, which, in turn, affects the degree of strain.

B. Conduction-band nonparabolicity parallel to the interface planes

Calculations of d^4E/dk^4 along the direction parallel to the interface planes have been performed with a variety of Si-$Si_{0.5}Ge_{0.5}$ superlattices in which the thicknesses of the silicon and alloy layers are not necessarily equal. The buffer layer in each case is assumed to have the same germanium and silicon concentrations as in the superlattice; thus a superlattice constructed of 18 monolayers of silicon atoms alternating with 2 monolayers of alloy atoms has a buffer layer of $Si_{0.95}Ge_{0.05}$. Calculations have also been performed with a Si-Ge superlattice system grown on a buffer of $Si_{0.5}Ge_{0.5}$.

The values in Table II represent the nonparabolicity near the position of the folded minimum on the superlattice axis. Since the calculations are performed along a direction parallel to the interface planes, this represents the direction of the transverse mass. As described in Sec. II, this minimum is lower in energy than the fourfold-degenerate minima, which have their major axis aligned parallel to the interfaces, and so is of more interest with regard to the transport properties. Since the lattice constant parallel to the interfaces is the same in each of the constituent layers (and is equal to the lattice constant of the buffer layer), the strained and unstrained models produce virtually identical results. The results quoted are those obtained with the strained model.

TABLE II. The values of d^4E/dk^4 for the ground-state conduction band of the strained system in the direction parallel to the interfaces. The results, in units of eV Å^4, are calculated at or near the position of the folded minimum on the superlattice axis, with the wave vector k being measured from the minimum.

		d^4E/dk^4
Si(5.5 Å)–$Si_{0.5}Ge_{0.5}$(5.5 Å)	$k=0$	2.0×10^3
Si(8 Å)–$Si_{0.5}Ge_{0.5}$(3 Å)	$k=0$	1.9×10^3
	$k=0$	2.1×10^3
Si(3 Å)–$Si_{0.5}Ge_{0.5}$(8 Å)	$k_x=0.01$	2.1×10^3
	$k_z=0.03$	2.0×10^3
Si(11 Å)–$Si_{0.5}Ge_{0.5}$(11 Å)	$k=0$	1.6×10^3
Si(14 Å)–$Si_{0.5}Ge_{0.5}$(14 Å)	$k=0$	1.0×10^3
	$k=0$	1.5×10^3
Si(24.5 Å)–$Si_{0.5}Ge_{0.5}$(3 Å)	$k_x=0.01$	1.5×10^3
	$k_z=0.03$	1.5×10^3
Si(3 Å)–$Si_{0.5}Ge_{0.5}$(24.5 Å)	$k=0$	1.8×10^3
Si(5.5 Å)–Ge(5.5 Å)	$k=0$	3.3×10^3
Si(14 Å)–Ge(14 Å)	$k=0$	1.8×10^3

From the results in Table II it can be seen that the values of d^4E/dk^4 for the Si-$Si_{0.5}Ge_{0.5}$ superlattices vary only by a factor of 2 between the smallest and largest results. In the Si-Ge systems the values of d^4E/dk^4 are again covered by a factor of 2, although the results are slightly larger than with Si-$Si_{0.5}Ge_{0.5}$ superlattices of similar structure. This is probably due to the increase in the confinement potential of the germanium barrier layer. There also appears to be a slight dependence on the period. The shorter lattices tend to have larger nonparabolicities, but with the small range of values available it cannot be stated whether this is a general rule. The results also show that the nonparabolicity does not change noticeably at wave vectors slightly away from the minimum.

The nonparabolicity along the parallel directions therefore appears to be fairly insensitive to changes in the superlattice parameters. This is in sharp contrast to the results along the superlattice axis, where variations in the period and movement away from the minimum cause order-of-magnitude changes in the nonparabolicity.

In the plane parallel to the interfaces, as in the bulk, virtual transitions between the lower conduction states are disallowed. Large matrix elements are, however, observed between the p-like conduction ground state and s-like states that are deep in the valence band. These states have energies at least 3 eV below the conduction-band edge, but the large transition probabilities cause them to dominate the nonparabolicity. Since the energy separation is large, the fourth derivative is fairly insensitive to small changes in the energy of these states, and this explains why the nonparabolicities are not greatly affected by changes in the superlattice parameters. The possibilities of enhancing the parallel nonparabolicity by engineering the energy bands seems to be rather limited.

C. Valence-band nonparabolicity

The results obtained in this subsection are for Si-$Si_{0.5}Ge_{0.5}$ superlattices with approximately equal barrier and well widths. In the "unstrained" model no adjustment was made to the pseudopotentials since confinement occurs in the alloy layers for both the strained and unstrained systems. A calculation in which the superlattice is filled with $Si_{0.5}Ge_{0.5}$ atoms is used as the bulk comparison.

The dispersion along the superlattice axis of the uppermost valence bands in the region of Γ is illustrated in Fig. 6.

The values of d^4E/dk^4 at the Brillouin-zone center Γ for the uppermost valence band are presented in Table III for directions along the superlattice axis and parallel to the interface planes. The range of values obtained with the strained superlattice cover an order of magnitude, but there is no obvious relation between the values of the fourth derivative and the variable parameters of the superlattices. The band curvature is principally due to virtual excitations between the valence band and the conduction states which lie about 2 eV above the conduc-

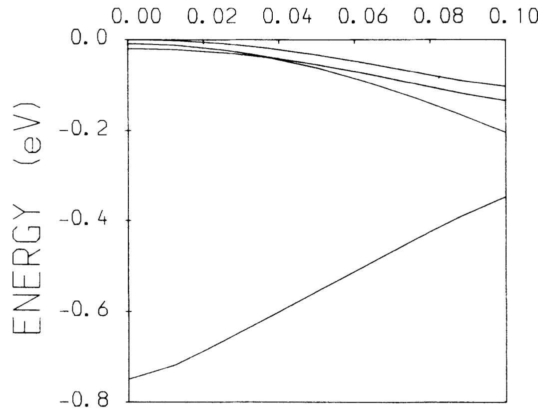

FIG. 6. Energy–vs–wave-vector dispersion relations for the four uppermost valence bands of a 22.0-Å-period Si-$Si_{0.5}Ge_{0.5}$ strained-layer superlattice. The dispersion is shown along the superlattice axis for the region near the Brillouin-zone center Γ. The wave vector k is measured in units of $2\pi/A$, where A is the lattice constant of the buffer layer $Si_{0.75}Ge_{0.25}$.

tion-band edge. There is also a small contribution from transitions within the valence band which is about an order of magnitude smaller than that from the conduction band and of opposite sign.

The unstrained superlattice calculations produce values of d^4E/dk^4 of the same magnitude as those from the strained superlattice, and the bulk value, of approximately -3×10^3 eV Å^4, is also in this range. Similar virtual transitions are responsible for the nonparabolicity in these cases. It can be concluded that the effects of strain and zone folding do not necessarily enhance the valence-band nonparabolicity; in fact, in some cases the nonparabolicity appears to be reduced. However, the fact that the results vary by an order of magnitude suggests that it may be possible to obtain an optimum nonparabolicity in a given direction by suitably selecting the superlattice parameters.

D. Effective masses

The effective mass m^* is given by second-order perturbation theory as

$$\frac{1}{m^*}=\frac{1}{m_e}+\frac{2}{m_e^2}\sum_{n\neq n'}\frac{|M_{nn'}|^2}{E_n-E_{n'}}\ , \qquad (8)$$

TABLE III. The values of d^4E/dk^4 at the Brillouin-zone center Γ for the valence-band edge along the directions parallel and perpendicular to the interface planes. The results are in units of eV Å^4.

		Perpendicular to interfaces	Parallel to interfaces
11.0-Å period	strained	-1.8×10^3	-9.6×10^3
22.0-Å period	strained	-3.5×10^3	-1.0×10^3
27.5-Å period	strained	-4.1×10^3	-2.1×10^3
	unstrained	-7.3×10^3	-5.3×10^3

where m_e is the free-electron mass. The values of the matrix elements $M_{nn'}$ and the energy separations $E_n-E_{n'}$ have already been discussed in the preceding subsections.

In the conduction band the masses of the fourfold-degenerate minima, in the [100] and [010] directions, are assumed to be bulklike.[1] In the twofold-degenerate minima it has been seen that strong virtual excitations exist in the superlattice that are not present in the bulk material and that significantly affect the band curvature. The longitudinal mass, along the superlattice axis, is found to be $0.54m_e$ and $0.35m_e$ in the 22.0- and 27.5-Å-period Si-$Si_{0.5}Ge_{0.5}$ strained superlattices, respectively. In comparison, when the superlattice is filled with silicon atoms to obtain the bulk result, a value of $1.0m_e$ is obtained, which is the expected value for a parabolic band. The superlattice effective mass is determined by virtual transitions involving the lower conduction states.

In the direction of the transverse mass the superlattice effective mass of $0.19m_e$ is virtually unchanged from the bulk value of $0.20m_e$ and appears to be unaffected by the superlattice period.

In the valence band the superlattice effective masses at the Brillouin-zone center, Γ of the band edge are calculated to be $0.21m_e$ and $0.17m_e$ in the directions parallel and perpendicular to the superlattice axis, respectively, for the 22.0-Å-period superlattice. The effective mass along the superlattice axis is found to vary slightly with the superlattice period, while the masses in the perpendicular directions are unchanged. When the superlattice is filled with $Si_{0.5}Ge_{0.5}$ atoms, a bulk value of $0.16m_e$ is obtained in each direction.

IV. DISCUSSION AND CONCLUSIONS

We have presented results concerning the band curvatures in Si-$Si_{1-x}Ge_x$ strained-layer superlattices with periods of 10–30 Å. The band curvature has been described qualitatively in terms of dispersion curves and the relevant virtual excitations, and quantitatively as effective masses and nonparabolicities (i.e., the second- and fourth-order derivatives of energy versus wave vector, respectively).

In the valence band the nonparabolicity and effective mass are approximately the same magnitude in the superlattice as in bulk $Si_{0.5}Ge_{0.5}$.

In the conduction band the differences between the superlattice and the bulk are far more noticeable. Along the superlattice axis three main differences are observed.

(i) The position of the minimum within the superlattice Brillouin zone varies as a function of the superlattice period.

(ii) The bulk minima are virtually parabolic, while in the superlattice the nonparabolicity is marked and is approximately equivalent to that in bulk GaAs.

(iii) The longitudinal effective mass in the superlattice is noticeably smaller than in the bulk.

The variation of the position of the minimum occurs because the bulk minima lie away from the high-symmetry points of the Brillouin zone. Therefore the position of the minimum along the superlattice axis is affected by the zone folding.

The differences in cases (ii) and (iii) above indicate that the curvature of the superlattice bands differ significantly from that predicted for the bulk material. This is due to the virtual transitions between the lower conduction states, which are allowed in the superlattice but not in the bulk. The importance of these terms in affecting the band curvature is enhanced by the small energy separations involved. The effective mass and the nonparabolicity are proportional to the inverse of the energy separation and to the inverse of the energy separation cubed, respectively. In the systems considered here the lowest two conduction states are separated by energies of between 10 and 200 meV, whereas transitions across the fundamental gap involve an energy change of at least 1 eV. Thus the virtual excitations between the conduction-band states dominate the band curvature. In fact, the nonparabolicity is so strongly dependent on the separation of the lower conduction states that the value can vary by 2 orders of magnitude for comparatively small changes in the superlattice parameters. This sensitivity suggests that "tuning" of the superlattice would be possible to obtain a desired value of nonparabolicity.

The effect of strain on the nonparabolicity of these structures is of great interest. We have shown that it is possible to estimate the band nonparabolicity with reasonable accuracy using a simple model in which the atoms occupy cubic lattice positions, as in the bulk material. In order to do this, the conduction-band edges of the constituent layers must be shifted relative to one another to reflect the potential barriers seen in the strained-layer superlattice. The full-scale strained-layer calculation is still needed in order to determine the required energy shift. The applicability of the simple model has only been demonstrated for the range of superlattices considered in this study, where the conduction-band nonparabolicity is dominated by the transition between the lower conduction states. To extend the use of the simple model to structures where this transition is not dominant would most probably lead to erroneous results since it has been demonstrated that certain transition probabilities, for example, those across the superlattice band gap, are severely underestimated in the simple model.

The conduction band parallel to the interface planes is also of interest due to the splitting by strain of the degenerate minima. The minima having their major axis along the superlattice axis are lowest in energy. Therefore, the electron transport parallel to the planes is determined by the minima along the superlattice axis, and so the relevant nonparabolicity is that measured in the direction of the transverse mass. The corresponding nonparabolicity is at least an order of magnitude less than in bulk GaAs, but is several orders of magnitude larger than the bulk Si value measured along the direction of the longitudinal mass.

It is interesting to compare these results with the conduction-band nonparabolicities obtained for GaAs-$Ga_{1-x}Al_xAs$ (Ref. 4) and GaAs-$GaAs_{1-x}P_x$ (Ref. 5). The principal differences can be summarized as follows.

(i) In the Si-$Si_{1-x}Ge_x$ system the minima are away from the major symmetry points, and therefore the position of the minimum within the superlattice Brillouin zone varies with the period, whereas the minimum in the GaAs systems is at Γ and so remains in this position.

(ii) The bulk GaAs conduction band is significantly nonparabolic, and the enhancement in the superlattice is less than an order of magnitude. The bulk-silicon conduction band is virtually parabolic near the extrema, but the effects of strain and zone folding enhance the nonparabolicity by many orders of magnitude, making it roughly equivalent to that of bulk GaAs.

(iii) The mechanism responsible for the conduction-band curvatures are considerably different in the three superlattice systems. In the silicon systems the nonparabolicity is entirely due to virtual transitions within the conduction band. These transitions are between states which originate from the same region of the bulk Brillouin zone, namely the minimum; therefore the overlap between these states is almost complete. The nonparabolicity of the GaAs-$Ga_{1-x}Al_xAs$ superlattices is also due solely to virtual transitions within the conduction band; however, the principal transitions are between the Γ minimum and the zone-folded states originating from the bulk X minimum. The overlap between these states and, therefore, the matrix element between them, is made finite by the momentum mixing of the superlattice potential. The GaAs-$GaAs_{1-x}P_x$ superlattices are strained, as in the Si-$Si_{1-x}Ge_x$ systems, to accommodate the lattice mismatch. The band curvature is affected by virtual transitions between the conduction states and across the superlattice band gap. For small concentrations of P the principal transition is again that between the Γ minimum and the folded X minimum. As the strain is increased, i.e., for larger concentrations of P, the momentum mixing is further enhanced, leading to an increase in the nonparabolicity. For x greater than about 0.53 the X minimum moves from the GaAs layer into the barrier, and the transition across the superlattice gap becomes dominant.

(iv) In directions parallel to the interface planes the band curvature in the GaAs superlattices is unchanged from that of the bulk material. In the silicon superlattices considered here, the strain splits the degenerate minima such that the minima along the superlattice axis are about 150 meV below those in other directions.[1] Consequently, the dispersion and, therefore, the band curvature, parallel to the interface planes is significantly different from that of the bulk material.

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