New Optical Transitions in Si-Ge Strained Superlattices

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Optical transitions in ultrathin Si-Ge strained superlattices are computed by means of a simple tight-binding model. The use of strain and folding arguments gives a clear understanding of the different origin of the transitions previously observed. The experimental dependence of intensities on the number of layers in the supercell is found to be a consequence of the fact that these superlattices are type II.

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Recent progress in silicon molecular-beam epitaxy[1,2] has made possible the growth of new systems where strained layers of the binary compound Ge_xSi_{1-x} are alternated with Si layers. An extremely interesting case is that of a superlattice (SL) where the binary compound becomes pure Ge. Ge layers grown on Si substrates have to undergo such an enormous strain that the system could be unstable. However, a recent paper[3] reports the growth on a (001)-oriented Si substrate of different SL $(Si)_n$-$(Ge)_n$, where the number n of layers of each component in the supercell is 1, 2, 4, or 6. The layers are so thin and the strains so large that these systems have been proposed as new semiconducting materials rather different from the binary compound. This is supported by the finding[3] of three unexplained direct transitions in the energy range between 0.7 and 2.4 eV when $n=4$, while the two lowest of these transitions are not observed for $n=6$.

The aim of this Letter is to show that the electronic structure of these materials can be easily understood in terms of the band structure of the constituents together with simple arguments on strain and zone folding. Kronig-Penney or envelope-function approaches seem to be unable to describe ultrathin $(Si)_n$-$(Ge)_n$ SL because folding makes states coming from the whole Brillouin zone of the host materials play an important role. The supercell is now small enough to try a self-consistent local-density calculation. However, such procedure requires an enormous amount of work to get the accuracy required for energy gaps and effective masses, on top of the difficulty introduced by the large spin-orbit coupling present in Ge. Therefore we use a tight-binding approach where all the ingredients can be included within a reasonable degree of practical complexity. We use an sp^3s^* basis with the two spin polarizations to represent the Hamiltonian H.[4] The first task to be accomplished is the description of strain effects on the bulk band structure. The deformation of the lattice has two consequences. The first one is a new angular distribution of the localized orbitals which can be very easily taken into account for s and p orbitals.[5] Since the s^* orbital is included to describe in an effective way the contribution coming from d states,[6] the angular dependence of their interactions is not clear at all. Therefore, we do not include any dependence on the deformation for the interactions involving s^*. The second effect is the change of interatomic distances d which is reflected in a scaling of the interactions. This aspect must be carefully treated for a good description of strain effects. Therefore we work with the scaling behavior self-consistently computed for Si and Ge.[7] In principle, a different scaling must be used for each interaction. All the off-diagonal interactions have a dependence close to d^{-2} so that we use this simple scaling for these matrix elements.[7] On the contrary, the behavior of the diagonal interactions $\langle s|H|s\rangle$ and $\langle p|H|p\rangle$ is quite different, being $d^{0.36}$ for Si and $d^{1.09}$ for Ge, the scaling we use here.[7] Since the scaling of $\langle s^*|H|s^*\rangle$ is not so clear[7] we use it as an adjustable parameter to obtain a good variation of the indirect band gap with hydrostatic pressure which brings us to a dependence of d^3 for both Si and Ge. To test the adequacy of this model for describing strain we compute hydrostatic, both direct (a^c-a^v) and indirect $(E_1+a^v)^\Delta$, and uniaxial (b and Ξ_u^Δ) deformation potentials[8-10] for Si and Ge. Table I shows our results together with experimental values[8] for comparison. The worst result is that for Ξ_u^Δ but it implies only an error of a few hundreths of an electronvolt in the bottom of the conduction band. The agreement is satisfactory, giving us confidence for using the model in the description of $(Si)_n$-$(Ge)_n$ strained SL.

The supercell of the SL grown on a (001) Si substrate has n Si atoms at their ideal bulk positions and n Ge

TABLE I. Theoretical and experimental values (in electronvolts) of selected deformation potentials of the Γ_8 valence bands and Γ_7 and Δ_1 conduction bands in Si and Ge.

	Si		Ge	
	Theory	Expt.	Theory	Expt.
(a^c-a^v)	−7.8	···	−8.5	−9.4[a]
b	−2.19	−2.27[a]	−3.1	−2.86[a]
Ξ_u^Δ	3.37	8.77[a]	4.37	···
$(E_1+a^v)^\Delta$	1.43	1.60[a]	1.32	···

[a]Reference 8.

atoms displaced to fit the Si lattice parameter in the (x,y) plane together with a change in the interplane distance in the z direction obtained from the Poisson ratio. The band structure is computed by direct diagonalization of a $(20n)\times(20n)$ Hamiltonian (five orbitals per atom plus spin-orbit interaction). We take the valence-band offset $\Delta E_v = 0.84$ eV from self-consistent calculations.[9] Since the SL we are concerned with are very thin, we have tested the possible effect of a nonabrupt potential shape. For $n=1$ and 2 the results are very dependent on the potential shape. Therefore we concentrate on the cases of $n=4$ and $n=6$ where the changes we obtain are in the range of some hundreths of an electronvolt but no qualitative differences appear. Figures 1 and 2 show the band structures of $(Si)_n$-$(Ge)_n$ strained SL along the k_z direction for $n=4$ and 6, respectively. The origin of energies is taken at the top of the Si bulk valence band (VB). The Si conduction bands (CB) folded into the SL Brillouin zone are included for clarifying the discussion. In these two figures it is possible to see how some CB of the SL closely follow the folded bottom of the Si CB. Moreover, in both figures one state appears around 2.5 eV which does not originate from these Si bands around the minimum in the Δ direction of the Brillouin zone. From the diagonalization of the Hamiltonian we get the eigenstates represented either in real space or in terms of bulk (unfolded) eigenstates as shown in Fig. 3 for $n=4$. In this way we conclude that the state close to 2.5 eV comes from the CB state at the Γ point of strained Ge. With the origin we have taken (top of the Ge strained VB at 0.84 eV) the strain has shifted the Ge Γ-like CB state up to 1.907 eV. The shift till its final energy position is due to SL effects. One can observe in Fig. 2 that for $n=6$ the Ge Γ-like state is very close in energy to bottomlike folded states, resulting in a set of mixed states in a narrow energy range. However, for $n=4$ (Fig. 1) such Ge Γ-like state lies far in energy from any folded bottomlike state. In order to compare with experimental information,[3] we compute transition probabilities[11] between the CB and the upper states of the SL VB, which are mainly Γ-like states in Ge as expected (i.e., these SL are type II; see Fig. 3). The key for the calculation of transition probabilities is the knowledge of the matrix elements of the momentum operator. Within a tight-binding scheme these matrix elements are written in terms of matrix elements of the Hamiltonian and distances between localized orbitals.[12] This gives satisfactory results[12] particularly in our case where just a comparison between different optical transitions is required. Figure 4 shows transitions probabilities between the ith CB state (C_i) and the jth VB state (V_j) computed at the Γ point of $(Si)_4$-$(Ge)_4$ and $(Si)_6$-$(Ge)_6$ SL. Because of the experimental linewidth, no resolution is possible between transitions C_iV_1 and C_iV_2. Therefore from the results in Fig. 4 only three transitions in the range 0.7–2.4 eV should be expected in the two SL we

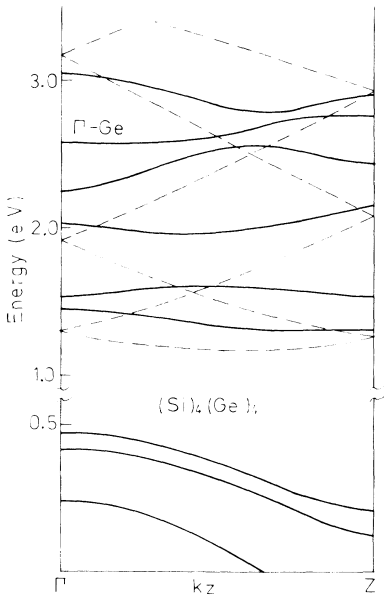

FIG. 1. Band structure (continuous line) of $(Si)_4$-$(Ge)_4$ strained SL along the k_z direction. Dashed lines are the Si CB folded into the SL Brillouin zone. The label Γ-Ge stands for the band with a large weight in bulk states of strained Ge at the center of the Brillouin zone.

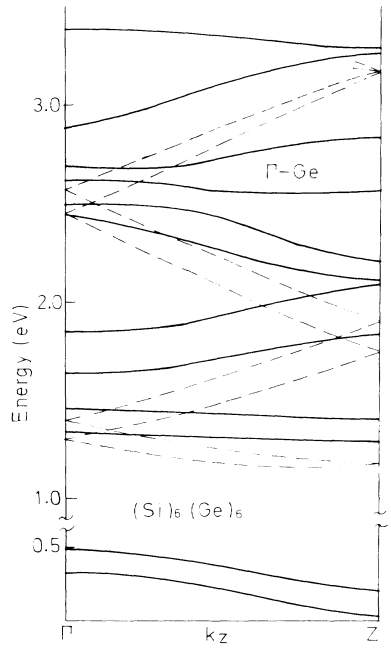

FIG. 2. Band structure (continuous line) of $(Si)_6$-$(Ge)_6$ strained SL along the k_z direction. Dashed lines are the Si CB folded into the SL Brillouin zone. The label Γ-Ge stands for the band with a large weight in bulk states of strained Ge at the center of the Brillouin zone.

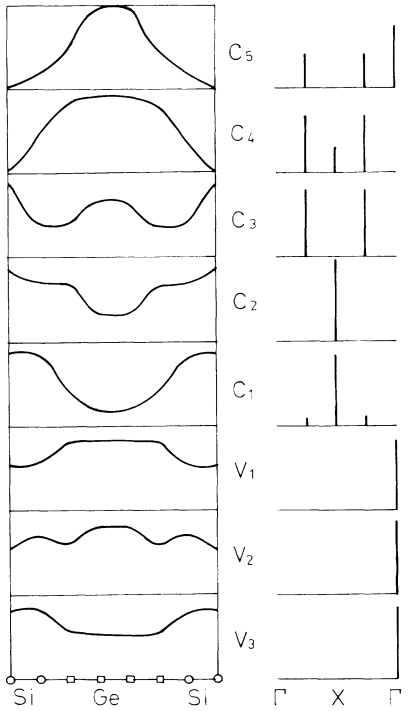

FIG. 3. Square of the wave functions of the states at the Γ point of a $(Si)_4$-$(Ge)_4$ SL as a function of tight-binding orbitals (left side) and of bulk eigenstates (right side). The states are ordered in increasing energy. The labels Γ, X, Γ, in the lower right side refer to bulk states in the extended Brillouin zone that contribute to the Γ states of the SL.

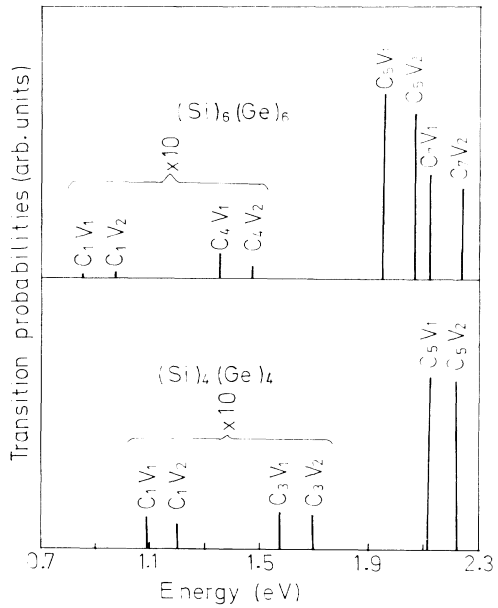

FIG. 4. Transition probabilities (in arbitrary units) between the ith CB state (C_i) and the jth VB state (V_j) computed at the Γ point of $(Si)_4$-$(Ge)_4$ and $(Si)_6$-$(Ge)_6$ SL. The intensity of the lowest-energy peaks has been multiplied by 10.

are concerned with. In both cases the transitions around 2.2 eV have the highest intensity because they originate from CB states with a large weight in the Γ bulk states. For $(Si)_6$-$(Ge)_6$ there are two CB states of this type as a result of the mixing mentioned above. The transitions with lower energy involve CB states originating from bulk bottomlike states (see Fig. 3). For $(Si)_4$-$(Ge)_4$ two transitions appear at 1.12 and 1.55 eV with intensities 0.016 and 0.020 relative to the intensity of the peak at 2.2 eV. For $(Si)_6$-$(Ge)_6$ this intensity relation further decreases to 0.002 and 0.007. This significant reduction explains why these two peaks are detected for $n=4$ while they are not for $n=6$.[3] For higher values of n the reduction is even greater because these SL are type II, having electrons and holes at different spatial regions. As far as the energy position is concerned, we get 1.12, 1.55, and 2.2 eV for the transitions in $(Si)_4$-$(Ge)_4$ in comparison with the experimental values 0.76, 1.25, and 2.31 eV. The only explanation we could find for the discrepancy in energy position is that the experiment is performed with a film of $(Si)_n$-$(Ge)_n$ with a thickness of only 50 Å width embedded in Si cladding layers. No significant confinement effects are expected because of the low barriers and high effective masses we have now. However, k_z is not a good quantum number anymore and transitions from the top of the SL VB at zone center Γ to states at the bottom of the SL CB at the zone edge Z become allowed. This reduces the transition frequencies of the two lowest peaks by roughly 0.2 eV (see Figs. 1 and 2) putting theory and experiment in better agreement.

In summary, the electronic structure of $(Si)_n$-$(Ge)_n$ strained SL can be easily understood by using a simple tight-binding model. The new set of transitions detected by electroreflectance,[3] as well as their behavior for varying n, are well accounted for by means of strain and folding concepts. We identify two different types of peaks regarding the origin of the CB state involved in the transition.

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$\lambda^{s.o.}=0.097$.

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