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Structural, electronic, and optical properties of strained $Si_{1-x}Ge_x$ alloys

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A systematic study of structural, electronic, and optical properties of strained $Si_{1-x}Ge_x$ alloys, coherently grown on a Si(001) surface, is presented. We find that for bulk alloys the lattice constant deviates from Vegard's law, while for the strained alloys it deviates from the results of elasticity theory. The strained alloys are indirect gap materials, with the minimum of the conduction band appearing in the [100] direction. We present results for the indirect as well as the direct gaps. Finally, we investigate the optical properties of strained alloys and present results for the critical energies as a function of the concentration of Ge in them.

I. INTRODUCTION

Recent developments in advanced epitaxial techniques (molecular-beam epitaxy, metal-organic depositions, etc.) have made possible the successful fabrication of strained $Si_{1-x}Ge_x$ alloys, Si/Ge superlattices, and multi-quantum-well systems and opened up the prospect of combining optic and electronic components of a device on the same substrate, the last being silicon, a material with highly advanced technology.[1–3] Besides the fabrication of optoelectronic devices, the strained $Si_{1-x}Ge_x$ alloys, coherently grown on silicon substrates, are also attractive candidates for the fabrication of advanced electronic devices, such as heterojunction bipolar transistors, resonant tunneling diodes, modulation-doped field-effect transistors, and so on.[4] For thin $Si_{1-x}Ge_x$ alloy layers, coherently grown on a Si substrate, the lattice constant in the plane of growth is determined by that of the substrate. The different lattice constants between the bulk $Si_{1-x}Ge_x$ alloys and the Si substrate lead to an inherent strain in the alloy layers, resulting in a significant modification of their band structure.

The first insights for the importance of strain in these materials were provided by Abstreiter and co-workers[5,6] and by People and co-workers.[7,8] People[7] estimated the band-edge shifts and splitting of strained $Si_{1-x}Ge_x$ alloys, in the range $0 < x < 0.75$, using linear deformation potential theory. Rieger and Vogl[9] have used nonlocal empirical pseudopotentials in order to calculate effective masses and deformation potentials. Ma *et al.*[10] presented an analysis of the symmetry properties of strained $Si_{1-x}Ge_x$ alloys grown on (001)-, (111)-, and (110)-oriented Si and Ge substrates. The purpose of the present work is to examine the electronic and optical properties of the strained $Si_{1-x}Ge_x$ alloys, coherently grown on a Si(001) surface. For the investigation of these alloys, we use an empirical tight-binding approach and give results in the entire Brillouin zone and for all alloy compositions $(0 < x < 1)$.

The interatomic distances in the strained $Si_{1-x}Ge_x$ alloys are an essential input to our calculations. In previous works the lattice constant of the bulk $Si_{1-x}Ge_x$ alloy was usually determined by Vegard's law[11], which is a linear interpolation between the lattice constants of Si and Ge,

$$a_0(x) = (1-x)a_{\rm Si} + x a_{\rm Ge}. \qquad (1)$$

For the strained $Si_{1-x}Ge_x$ alloys, grown coherently on a Si(001) surface, the lattice constant perpendicular to the growth plane was usually obtained from elasticity theory by a minimization of elastic energy, resulting in the expression[11,12]

$$a_\perp(x) = a_0(x)\left(1 - \frac{2C_{12}(x)}{C_{11}(x)}\frac{a_{\rm Si} - a_0(x)}{a_0(x)}\right), \qquad (2)$$

where $C_{11}(x)$ and $C_{12}(x)$, the elastic constants for the alloy, had been obtained by linear interpolation to those of bulk Si and Ge. However, as early as 1964,[13] deviations from Vegard's law were experimentally detected. The measured[13] lattice constant for bulk $Si_{1-x}Ge_x$ alloys can be represented by the expression[9] (in Å)

$$a_0(x) = a_{\rm Si} + 0.200x(1-x) + (a_{\rm Ge} - a_{\rm Si})x^2. \qquad (3)$$

Since the interatomic distances do play an important role in the determination of electronic and optical properties of alloys, we have also investigated the lattice constant of the bulk as well as the strained $Si_{1-x}Ge_x$ alloys.

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TABLE I. Lattice constant (in Å) for bulk $Si_{1-x}Ge_x$ alloys.

x	0.0	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1.0
$a_0(x)$	5.432	5.454	5.475	5.497	5.519	5.542	5.565	5.587	5.610	5.633	5.657

The paper is organized as follows. Section II deals with the determination of the structure of the bulk as well as the strained $Si_{1-x}Ge_x$ alloys. In Sec. III the electronic properties of the strained alloys are analyzed. Section IV deals with the determination of the corresponding optical properties. Finally, in Sec. V we summarize our findings and give our conclusions.

II. STRUCTURE

Modeling the interatomic forces in strained $Si_{1-x}Ge_x$ alloys is not an easy task because of the considerable strain fields that are present (even the relaxed bulk alloys have considerable strain energies[14]). Here a reliable description of the energetics is provided by using a semiempirical interatomic potential for Si-Ge systems,[15] which treats strain and heteronuclear bonding reasonably accurately and which has been well tested.[16,17] The form of the model is a direct generalization of that for the elemental systems Si and Ge. The present semiempirical approach is in principle less accurate than an *ab initio* determination of interatomic forces and total energies. It gives us, however, the opportunity to extensively relax our structures and use supercells with a large number of atoms. On the other hand, *ab initio* calculations are limited to small numbers of atoms and often suffer from incomplete relaxations or from inadequate plane-wave cutoff energies and **k**-point sampling. In any case, our results for bulk SiGe phases compare favorably, regarding both prediction of energies as well as of elastic constants, with extensive and systematic first-principles pseudopotential calculations.[14]

We first examine the lattice parameters of the relaxed random alloy. Table I presents the results of our calculations for the lattice constants of the bulk $Si_{1-x}Ge_x$ alloy, as a function of x. A comparison of these results to experimental data as well as to lattice constants determined by Vegard's law is illustrated in Fig. 1. Our results can be described by the expression (in Å)

$$a_0(x) = a_{Si} + 0.214x + 0.0105x^2, \tag{4}$$

while the experimental data are described by Eq. (3). Our calculations imply a deviation from Vegard's law and a bowing to the behavior of $a_0(x)$, in agreement with the experimental data. There exists, however, a small but systematic difference between our results on this bowing and the experimental data, especially for intermediate values of x (our results show less bowing than experiment). The origin of this small discrepancy may lie in an insufficient description, by the present empirical potential, of the observed[18] bowing in the elastic constants with alloy composition. (The same insufficient description is even reported by pseudopotential calculations.[14]) We also cannot exclude the possibility that a small ambiguity in the experimental determination of the concentration x of Ge in the alloy could partly account for this difference. A very accurate determination of the composition of the alloy would therefore be needed in order to check possible deviations between our results and the experimental data. Small deviations from Vegard's law have also been found previously,[19] but they had not been compared to the experimental data.

We turn now to the study of the structure of the strained $Si_{1-x}Ge_x$ alloys coherently grown on a Si(001) surface, where the lattice constant in the growth plane is equal to that of the substrate. Our results for the perpendicular lattice constant are presented in Table II and can be described by the expression (in Å)

$$a_{\perp}(x) = a_{Si} + 0.4005x - 0.0063x^2. \tag{5}$$

A comparison between these results and those of the elasticity theory Eq. (2) is given in Fig. 2. We observe in our results a small deviation from the predictions of elasticity theory. This "epitaxial bowing" is consistent with that found above for the bulk alloys. At $x = 1$, i.e., for epitaxial Ge, our predicted epitaxial lattice constant is slightly smaller than the result from elasticity theory (≈ 0.01 Å). This is in agreement with previous results from pseudopotential calculations.[14,20,21]

III. ELECTRONIC PROPERTIES

The calculations are based on the virtual crystal approximation with an empirical tight-binding model Hamiltonian with an sp^3 set of orbitals, including spin-

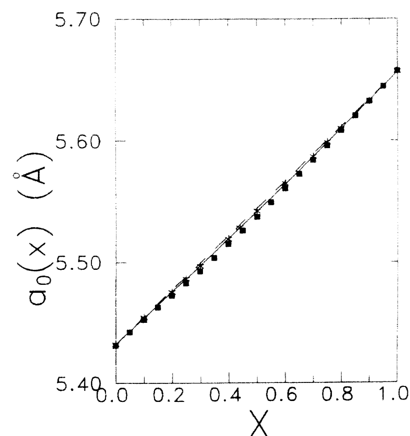

FIG. 1. Variation of the lattice constant of bulk $Si_{1-x}Ge_x$ alloys with x, according to calculations of the present work (asterisks), Vegard's law (dashed line), and the experimental measurements of Dismukes *et al.* (Ref. 13) (squares). The solid line represents Eq. (4).

TABLE II. Perpendicular lattice constant (in Å) for strained $Si_{1-x}Ge_x$ alloys.

x	0.0	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1.0
$a_\perp(x)$	5.432	5.476	5.517	5.559	5.597	5.636	5.673	5.710	5.764	5.780	5.813

orbit interaction.[22] The three-center representation and third-neighbor interactions are used in order to obtain both a good description of the valence and lower conduction bands and good values for the deformation potentials as well. The interaction parameters are fitted to reproduce the properties of the constituent bulk materials. A consequence of the lattice deformation is a change in the distances between the atoms and a modification of the bond angles. The first effect produces a change in the nondiagonal Hamiltonian integrals and is taken into account by using a scaling formula

$$H_{\alpha,\beta}(d) = H_{\alpha,\beta}(d_0)(d_0/d)^{\nu}, \tag{6}$$

where α, β represent atomic orbitals and d_0, d the bulk and strained interatomic distances, respectively. The number ν takes the value 3 for the s-s interaction and 1.8 for the s-p and p-p interactions.[22] The effect of the bond angle modification is taken into account by using the relations between the three-center and two-center integrals. The tetragonal crystal field splitting of p orbital energies is also taken into account.

For strained $Si_{1-x}Ge_x$ alloys coherently grown on a Si(001) substrate the space group of the distorted lattice is[10] D_{4h}^{19}. The sixfold degenerate conduction band minima $\Delta(6)$ for bulk alloys are split by the strain into twofold degenerate $\Delta(2)$ minima lying perpendicular to the growth plane and fourfold degenerate $\Delta(4)$ minima parallel to the growth plane. Also the heavy-hole (hh) and light-hole (lh) states at Γ are split by the lateral strain. For growth on a Si(001) substrate the $\Delta(2)$ minima are lying at higher energies than the $\Delta(4)$ minima and the hh states moves to higher energies than the lh states. In Fig. 3 the band structure of the strained alloy $Si_{0.5}Ge_{0.5}$, coherently grown on a Si(001) surface, is shown. These results imply that we are dealing with an indirect gap material with the fundamental gap at the point $k \cong 0.85(2\pi/a)$ along the $\langle 100 \rangle$ direction and having the value $E_g^i[\Delta(4)] = 0.82$ eV. Figure 4 shows the variation of the direct $E_g^d(\Gamma)$ and indirect gaps along the $\langle 100 \rangle$ and $\langle 001 \rangle$ directions, $E_g^i[\Delta(4)]$ and $E_g^i[\Delta(2)]$, respectively, and at the N point, $E_g^i(N)$, as a function of x, for the strained alloys $Si_{1-x}Ge_x$, coherently grown on a Si(001) surface. From this figure we deduce that all these are indirect gap materials. Contrary to the unstrained $Si_{1-x}Ge_x$, where the fundamental gap for $0 < x < 0.85$ ($0.85 < x < 1$) is along the $\langle 100 \rangle$ direction (at the L point),[23–25] the fundamental gap of the strained alloy coherently grown on a Si(001) surface is always along the $\langle 100 \rangle$ direction. Even though the value of the gap at point N reduces rapidly with x, it never becomes smaller than the one along the $\langle 100 \rangle$ direction. The gap along the $\langle 100 \rangle$ direction reduces with x, while the one along the $\langle 001 \rangle$ increases with it. For $0 < x < 0.7$ ($0.7 < x < 1$) the gap along the $\langle 001 \rangle$ direction is smaller (larger) than the gap at point N. The direct gap at Γ is always larger compared to the previously mentioned gaps. The break in the variation of the direct gap at $x = 0.3$ comes from the fact that for $x < 0.3$ the bottom of the conduction band at Γ is the Γ_6^- state, while for $x > 0.3$ it is the Γ_7^- state.

Finally, Fig. 5 shows the band gap between the two top valence bands (hh and lh states) and the bottom of the conduction band $[\Delta(4)]$ state. In the same figure are shown also the experimental data at 90 K of 75 Å and 33 Å of $Si_{1-x}Ge_x$/Si wells, after correcting for quantum well shifts, of Ref. 8 . Our calculations predict correctly the behavior of the gaps, but there exists a difference between the calculated values and the experimental data.

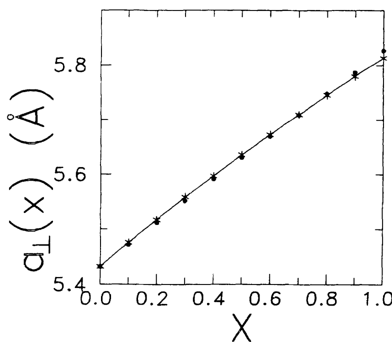

FIG. 2. Variation with x of the perpendicular lattice constant of strained $Si_{1-x}Ge_x$ alloys, coherently grown on a Si (001) surface, according to calculations of the present work (asterisks) and the elasticity theory (dots). The solid line represents Eq. (5).

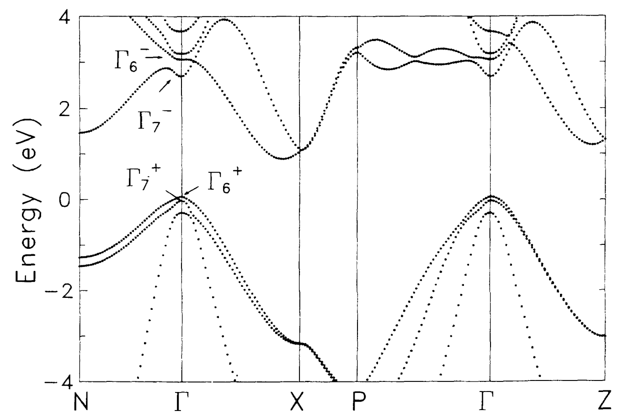

FIG. 3. Band structure of the strained alloy $Si_{0.5}Ge_{0.5}$ coherently grown on a Si (001) surface.

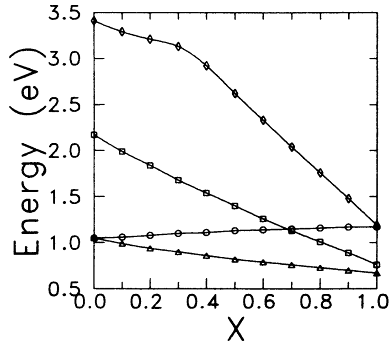

FIG. 4. Band gaps of strained $Si_{1-x}Ge_x$ alloys, coherently grown on a Si(001) surface, as a function of x. The indirect gaps $E_g^i[\Delta(4)]$ ($\triangle$), $E_g^i[\Delta(2)]$ ($\circ$), and $E_g^i(N)$ ($\square$), as well as the direct $E_g^d(\Gamma)$ ($\diamond$) gap, are shown.

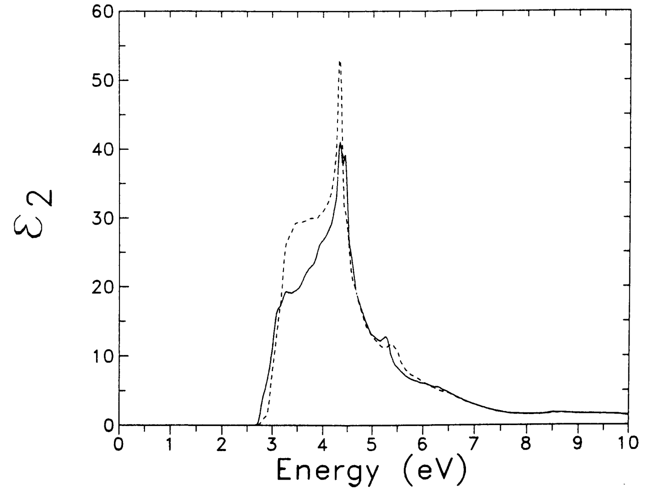

FIG. 6. Imaginary part ε_2 of the dielectric function of the strained $Si_{0.5}Ge_{0.5}$ alloy.

IV. OPTICAL PROPERTIES

Investigation of the optical properties of materials requires knowledge of the dielectric functions. The details of the method used for the calculation are presented in Ref. 22. We should point out that only direct transitions are taken into account, without the inclusion of phonons, excitons, etc. Figure 6 shows the imaginary part of the dielectric function ε_2 for the strained $Si_{0.5}Ge_{0.5}$ alloy. The consequence of the crystal symmetry D_{4h}^{19} is an anisotropy parallel and perpendicular to the growth plane. This anisotropy between the (x,y) plane and the z axis is significant only for energies smaller than 4.5 eV; for higher energies the anisotropy in ε_2 practically diminishes. In addition, a splitting of the peak E_2 in ε_2 appears.

Figure 7 shows the critical energies E_0, $E_0+\Delta_0$, E_1, $E_1+\Delta_1$, and E_0', as extracted from the band structure of the strain $Si_{1-x}Ge_x$ alloys, coherently grown on a Si(001) surface, as a function of x. E_0 comes from transitions at Γ between the highest valence band and the conduction state Γ_7^-, $E_0+\Delta_0$ from transitions between the spin split-off band and the conduction Γ_7^- state, and E_0' from transitions between the highest valence band and the Γ_6^- state. The E_1 ($E_1+\Delta_1$) structure comes from excitation near the N point between the highest (second highest) valence band and the lowest conduction band. The rapid variation of E_0 and $E_0+\Delta_0$ with x comes from the corresponding rapid variation of the energy of the state Γ_7^-. The smaller variation with x of the state Γ_6^- implies a smaller variation of the critical energy E_0'. The critical energies E_1 and $E_1+\Delta_1$ show a variation similar to that of E_0'.

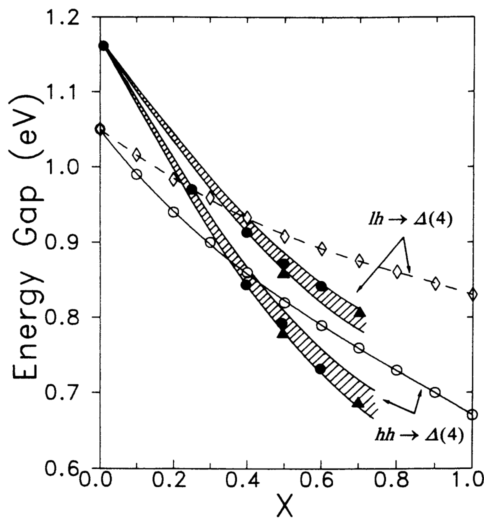

FIG. 5. Band gaps between the hh and lh states and the $\Delta(4)$ conduction band state for strained $Si_{1-x}Ge_x$ alloys, coherently grown on a Si(100) surface, as a function of x. The calculations ($\bigcirc$ and $\diamond$) show the strain-split valence bands. The experimental data at 90 K for 75 Å ($\bullet$) and 33 Å $Si_{1-x}Ge_x$/Si wells ($\blacktriangle$) (Ref. 8), after correcting for quantum well shifts, are also shown.

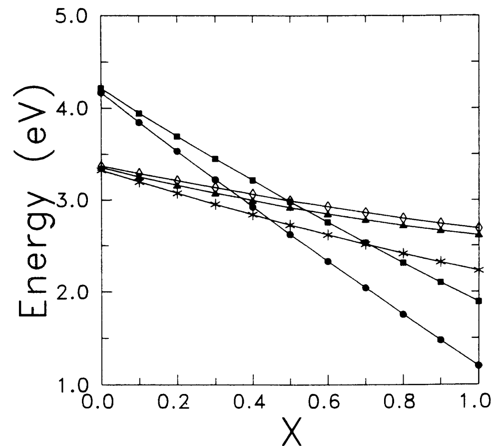

FIG. 7. Critical energies E_0 (full circles), $E_0+\Delta_0$ (full squares), E_1 (asterisks), $E_1+\Delta_1$ (full triangles), and E_0' (open diamonds) as a function of x for the strained $Si_{1-x}Ge_x$ alloys.

V. CONCLUSIONS

We have presented a systematic study of the structural, electronic, and optical properties of strained $Si_{1-x}Ge_x$ alloys, coherently grown on a Si(001) surface. We have calculated the lattice constants of bulk as well as strained alloys and found a nonlinear behavior and deviations from Vegard's law and the theory of elasticity. The results of our calculations for the lattice constant of the bulk $Si_{1-x}Ge_x$ alloys are given in Table I and can be described by the expression (in angstroms)

$$a_0(x) = a_{\rm Si} + 0.214x + 0.0105x^2. \quad (7)$$

For the strained $Si_{1-x}Ge_x$ alloys coherently grown on a Si(001) surface, the lattice constant in the growth plane is equal to that of the substrate. With regard to the perpendicular lattice constant the results of our calculation are summarized in Table II and can be described by the expression (in Å)

$$a_\perp(x) = a_{\rm Si} + 0.4005x - 0.0063x^2. \quad (8)$$

Concerning the electronic properties of the strained alloys, our investigation showed that they are indirect gap materials, with the fundamental gap always along the $\langle 100 \rangle$ direction, near the $k \cong 0.852\pi/a$ point. The variation of the indirect gaps along the $\langle 100 \rangle$, $\langle 001 \rangle$, and $\langle 111 \rangle$ directions, as well as the direct gap at Γ, were investigated and the results presented in Fig. 4. Finally the optical properties of strained $Si_{1-x}Ge_x$ alloys, coherently grown on a Si(001) surface, were studied via the calculation of the imaginary part of the dielectric function. The variation of critical energies with x is shown in Fig. 7.

ACKNOWLEDGMENT

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