Quantification of the strain in fully relaxed Si/Ge heteroepitaxial films and superlattices via molecular dynamics

D. Srivastava, R. S. Taylor, and B. J. Garrison
Department of Chemistry, The Pennsylvania State University, University Park, Pennsylvania 16802

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The fully relaxed Si/Ge heteroepitaxial films are simulated via molecular dynamics with Tersoff's potential for Si–Si, Si–Ge, and Ge–Ge interactions. The lattice mismatch induced strain is computed as a function of the thickness of the film. The strain values of the bulk Si and Ge layers are found to be in excellent agreement with those obtained via *ab initio* local density functional calculations. In thick uncapped epitaxial films, we find that the surface reconstruction induced relaxations significantly alter the strain values in the top five layers. When the film is less than five layers thick, we show for the first time that these relaxations do not cross the Si/Ge interface but are fully contained within the epitaxial film region. For all of the geometries studied, it has been found that at the Si/Ge interface, the adjacent Ge layer moves towards the interface and the adjacent Si layer moves away from the interface. Though very small in magnitude, these additional relaxations significantly alter the generally assumed geometries of the Si_2Ge_2/Si{001}, Si_4Ge_4/Si{001}, Si_3Ge_1/Si{001}, and Si_1Ge_3/Si{001} superlattices.

I. INTRODUCTION

Heterostructures provide a new class of materials which have potentially useful optical and electronic properties. Si/Ge heterostructures have recently received considerable attention due to the ease with which they can be directly integrated into existing silicon technology.[1]

The 4.2% lattice mismatch which exists between crystalline Si and Ge causes a strain in epitaxial Si/Ge heterostructures. Due to this strain, only ultrathin defect-free films of Ge on Si (or of Si on Ge) can be grown. Defect-free films of Ge of up to six layers[2,3] on the (2×1)-Si{001} surface and of up to four layers[3] on the (7×7)-Si{111} surface have been grown successfully. Also, defect-free films of Si on Ge{001} have been grown up to a thickness of four layers.[4] By controlling the growth rate to the precision of a few hundredths of a layer, it is possible to grow heterostructures (superlattices) with alternating layers of Si and Ge on the Si{001} surface.[2] The synthesis of these superlattices by molecular-beam epitaxy (MBE) is based upon the premise that at low temperatures, the growth structures are thermodynamically stable or metastable and that the ordering processes are driven primarily by the strain in the epitaxial film.[5,6] The effects of the strain on the electronic[7] and optical[8] properties of the superlattices are well established. In systems where strained-Ge (*s*-Ge) has been grown epitaxially on the {001} surface of unstrained Si, local density functional (LDF) calculations show that the indirect band gap is lowered.[7] Whereas, in systems where strained-Si (*s*-Si) has been grown on the {001} surface of unstrained Ge, LDF calculations indicate that a direct band gap may exist.[8] Thus, these superlattices may be suitable for optical device fabrication. The experimental studies to quantify the strain in ultrathin (two to ten layer) epitaxial *s*-Ge and *s*-Si films have been attempted only recently.[4,9] Computer simulations based upon LDF calculations of the Si/Ge interface in bulk[9–11] and upon simple geometric considerations[4] based on continuum elastic theory are used to explain the experimental results. It is not clear, however, that the strain in the ultrathin films can be described quantitatively using the macroscopic theories associated with the Si/Ge interface in bulk.

Using Tersoff's many-body potential[12] for Si, Ge, and SiGe in a direct simulation, we have constructed four different configurations of Si/Ge heteroepitaxial films. Two of these have *s*-Ge supported epitaxially on unstrained Si{001} (*s*-Ge/Si and Si/*s*-Ge/Si), and the other two have *s*-Si supported on unstrained Ge{001} (*s*-Si/Ge and Ge/*s*-Si/Ge). We allow these systems to fully relax; i.e., the geometry is optimized as according to Tersoff's potential to give us the lowest energy configuration for each case. During these relaxations, we have not observed the formation of any dislocations or other defects. The strain in the germanium and silicon epilayers is evaluated by comparing the values of the perpendicular lattice constants, $a_\perp^{s\text{-}Si}$ and $a_\perp^{s\text{-}Ge}$, with the corresponding equilibrium unstrained perpendicular lattice constants, $a_\perp^{Si}$ and $a_\perp^{Ge}$. The strain values we have calculated for the bulk Si and Ge layers and for the bulk Si/Ge interface are in excellent agreement with those obtained from LDF calculations and macroscopic elastic theories.[11] In the uncapped *s*-Ge/Si{001} and *s*-Si/Ge{001} epitaxial films, we find that the relaxations induced by the (2×1)-dimer reconstruction of the surface layer significantly alter the strain values of the top five epitaxial layers. When the film is less than five layers thick, however, these surface reconstruction induced relaxations do not cross the Si/Ge interface but are restricted to the epitaxial film region. For epitaxial films less than five layers thick, the effects of the surface reconstructions on the

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film are found to be substantial and should not be ignored in the interpretation of the experimental results.[4] In both the strained Ge and strained Si systems, we find that at the Si/Ge interface the adjacent Ge layer relaxes toward the interface and the adjacent Si layer relaxes away from the interface. Though very small in magnitude, these relaxations significantly alter the generally assumed geometries of the Si_2Ge_2/Si{001}, Si_4Ge_4/Si{001}, Si_3Ge_1/Si{001}, and Si_1Ge_3/Si{001} superlattices. The perpendicular lattice constants of these fully relaxed superlattices are calculated and are compared to those reported in some other recent works.

The simulation method used is described in Sec. II. The results for the *s*-Ge/Si heterostructures are given in Sec. III A. Sections III B and III C contain the results for the *s*-Si/Ge heterostructures and Si_nGe_m superlattices, respectively. A discussion of how these results relate to those obtained from LDF calculations and experimental measurements is given in Sec. IV.

II. METHOD

Uniaxially strained epitaxial films of Ge on Si{001} and of Si on Ge{001} and Si–Ge superlattices are constructed using the quasimolecular dynamics method[14] and Tersoff's many-body potential for two component Si–Ge systems.[15] The parameterization of Tersoff's potential has been specifically optimized for describing the elastic properties of Si, Ge and SiGe.[12,15] Hence, this potential should provide a good description of the strain which is present in Si/Ge heterostructures and superlattices. We note that we have previously used Tersoff's potential in molecular dynamics simulations of the epitaxial growth of several layers of Si and of Ge on the (2×1)-Si{001}[16,17] surface, and that we have found that the strain existing in the first few epitaxially deposited Ge layers is comparable to that found in LDF and elastic theory studies.[11]

The perpendicular lattice constants are obtained for two different film configurations of strained Ge and strained Si heterostructures and for four different Si/Ge superlattices. The first type of Si/Ge heterostructure is shown in Fig. 1(a), where a *s*-Ge (*s*-Si) film is epitaxially supported on a six layer thick Si (Ge) substrate. The thickness of the epitaxial film is systematically varied from two layers, where the first Ge (Si) layer is at the interface and the second Ge (Si) layer has a (2×1)-dimer reconstruction, to ten layers where eight additional bulk *s*-Ge (*s*-Si) layers have been inserted between the interfacial and the dimer reconstructed layer. In the second type of Si/Ge heterostructure [Fig. 1(b)], a two to ten layer thick *s*-Ge (*s*-Si) epitaxial film is capped on both sides with six layers of unstrained Si (Ge). For the superlattices, alternating films of Ge and Si are supported epitaxially on a six layer silicon substrate. In both the heterostructures and the superlattices, the bottom layer is held fixed and the top layer has a (2×1)-dimer reconstruction. All of the atoms in the simulation are initially given lattice sites corresponding to the pure unstrained system. The periodic boundary conditions parallel to the {001} surface plane maintain the horizontal lattice constant to be that of the unstrained substrate; whereas, in the plane perpendicular to the {001} surface the crystal is allowed to relax freely via the forces derived from Tersoff's potential. This is done by heating[18] the crystal to 1000 K for a period of approximately 10 ps (1 ps = 10^{-12} s) during which time the atoms move to

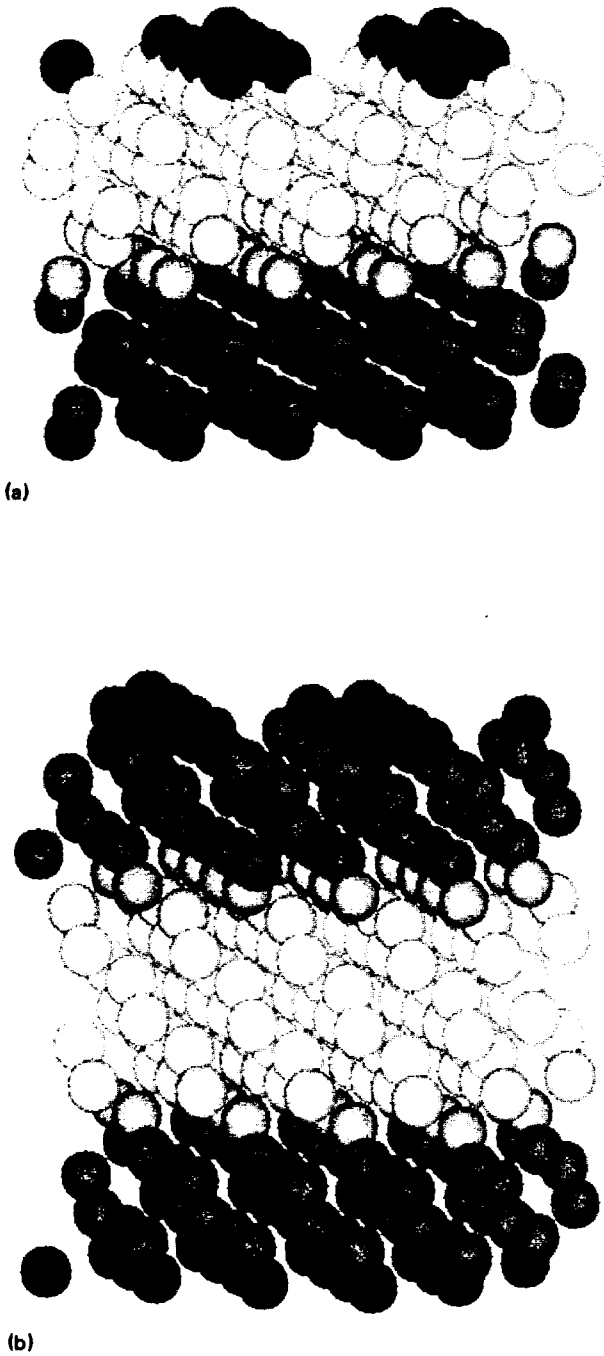

FIG. 1. Three-dimensional pictures of the Si/Ge heteroepitaxial systems. (a) *s*-Ge/Si{001} system with a six layer (16 atoms/layer) thick Ge epitaxial film on a Si{001} substrate. The substrate Si atoms are grey and the bulk Ge atoms in the epitaxial film are white. The rigid bottom layer Si atoms are black and the (2×1)-reconstructed Ge atoms are charcoal grey. (b) the same as (a) except that the Ge epitaxial film is sandwiched between two six layer films of Si atoms. Here the (2×1)-reconstruction is on the top Si layer. The *s*-Si/Ge systems are analogous.

positions corresponding to a lower energy configuration. This system is then evolved for an additional 10 to 40 ps during which if the kinetic energy of an atom reaches a maximum, its velocity is set to zero.[14] In this manner, the sample is cooled to near 0 K. Convergence is achieved by heating the crystal to different temperatures and then quenching it until all of the kinetic energy is removed. The interlayer spacings, $d_\perp$, calculated from the final equilibrium configurations are used to compute the perpendicular lattice constants, $a_\perp$, for the strained system.

III. RESULTS

Included in this section are the results of the calculations for the different types of Si/Ge heteroepitaxial systems and superlattices. Sections III A and III B contain the results for the strained Ge and strained Si heteroepitaxial films, respectively. The results of the simulations on the Si_2Ge_2, Si_4Ge_4, Si_3Ge_1, and Si_1Ge_3 superlattices are given in Sec. III C.

A. Strained Ge in *s*-Ge/Si{001} and Si/*s*-Ge/Si{001} heterostructures

For the uncapped *s*-Ge/Si{001} system, shown in Fig. 1(a), we have plotted the perpendicular lattice constant as a function of three different film thicknesses in Fig. 2. Instead of using the interlayer spacings $d_\perp$ we have chosen to plot the lattice constant normal to the {001} plane, $a_\perp = 4d_\perp$, because these values are easier to interpret when compared with the equilibrium bulk lattice constants of Si, $a^{Si} = 5.43$ Å, and of Ge, $a^{Ge} = 5.65$ Å. Starting from the left on the abscissa, the first six layers are of unstrained Si and those labeled eight or larger are of uniaxially strained Ge. The lattice constant of the *s*-Ge/Si interface is plotted at the seventh layer. First, we consider a ten layer thick Ge epitaxial film. The perpendicular lattice constant corresponding to the unstrained Si layers, a_1^{Si}, (layer positions four and five) is 5.433 Å. The bulk *s*-Ge layers in the epitaxial film (layer positions nine to twelve) have $a_1^{s\text{-}Ge} = 5.816$ Å. The lattice constant at the *s*-Ge/Si interface, $a_1^{s\text{-}Ge/Si}$, (layer position seven) is 5.631 Å. These results agree well with those, $a_1^{s\text{-}Ge} = 5.82$ Å (as indicated by the dotted line in Fig. 2) and $a_1^{s\text{-}Ge/Si} = 5.62$ Å, obtained via elastic theory and LDF calculations for bulk *s*-Ge/Si heterostructures.[11] Deviations from the elastic theory occur in the additional relaxations of the Si and Ge layers adjacent to the interface. At layer position six, we note that the lattice constant for Si is 0.014 Å smaller than the corresponding value at layer positions four and five. Similarly, at layer position eight, the perpendicular lattice constant for the *s*-Ge is 0.017 Å larger than that of the bulk-like *s*-Ge in layers nine through twelve. Upon a detailed examination of the interface, we find that this is due to a 0.004 Å relaxation of the Ge layer toward the interface and a 0.004 Å relaxation of the Si layer away from the interface. In other words, both the Si and Ge layers at the interface move towards the silicon. These additional relaxations are not affected by the surface reconstructions and are not dependent upon the thickness of the epitaxial film. Even though the magnitude of these additional relaxations is small, their effect on the band gap properties of Si–Ge superlattices when the repeat period of the superlattice is on the order of two to four layers, could be significant and will be discussed below. Similar relaxations of the Si and Ge layers adjacent to the Si/Ge interface have been found in the recent LDF calculations of Froyen, *et al.*[19] and Ciraci and Batra.[13] Originally, these authors[13] ignored the effects of these relaxations on the band gap properties of Si–Ge superlattices. Recently, however, the additional relaxations of the interfacial layers have been taken into account in band structure calculations.[20]

The effect of the surface reconstruction on the underlying strained epitaxial film manifests itself mainly in the inward relaxation of the top reconstructed *s*-Ge layer and the outward relaxation of the next inner *s*-Ge layer. The average inward relaxation of the top reconstructed *s*-Ge layer in the epitaxial film is 0.07 Å, while the average outward relaxation of the next layer is 0.03 Å. This causes the perpendicular lattice constants at layer position sixteen to be 6.8% smaller and at layer position fifteen to be 2.3% larger than those of the other epitaxial Ge layers. The perpendicular lattice constants at layer positions thirteen and fourteen also show small deviations from the average bulk strain value of $a_1^{s\text{-}Ge} = 5.816$ Å. These deviations are also due to the surface reconstructions. Thus, we note that the effects of the surface reconstructions extend as deep as five layers into the epitaxial film. The surface reconstruction induced relaxations of the top layers in the strained epitaxial film are generally quite different from those in an unstrained epitaxial films. For example the inward relaxation of the top *s*-Ge layer (0.07 Å) is much smaller than corresponding relaxation of the top unstrained Ge layer (0.14 Å).

In Fig. 2, we have also shown the similar variations in the values of the perpendicular lattice constants for two and four layer thick strained Ge epitaxial films. In both cases, we note that (i) the Ge (Si) layer adjacent to the *s*-Ge/Si interface shows about a 0.30% relaxation towards (away from) the interface, and that (ii) the effect of the surface reconstruction induced relaxations in the strained Ge layers deviates from the corresponding effect in unstrained Ge layers. For all three cases shown in Fig. 2, we note, however, that the perpendicular lattice constant for the Si layers is not affected by the surface reconstructions. Specifically, for a two layer

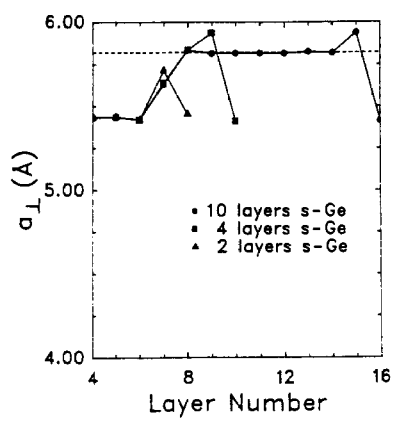

FIG. 2. The variations in the perpendicular lattice constant ($a_\perp$) vs the layer number for a ten layer thick (●), a four layer thick (■), and a two layer thick (▲) strained-Ge epitaxial film in the *s*-Ge/Si{001} system [Fig. 1(a)]. The dotted line indicates the *s*-Ge lattice constant as predicted by continuum elastic theory.

thick Ge epitaxial film, it is seen for the first time that the effects of the surface reconstructions do not extend five layers deep into the crystal; i.e., all of the relaxations due to the surface reconstructions are restricted to the Ge epilayers.

Figure 3 shows a similar study of the magnitude of the strain as a function of the Ge film thickness for the capped Si/*s*-Ge/Si{001} system which is depicted in Fig. 1(b). Again we show the results for a two, four, and ten layer thick epitaxial *s*-Ge film. In contrast to the previous simulation, there are now two interfaces. In Fig. 3, we have shown only the variation in the perpendicular lattice constant about the interface between the substrate and the epitaxial Ge film. The variation in the lattice constant in going from the *s*-Ge epitaxial film into the unstrained Si cap is symmetric to that of going from the *s*-Ge epitaxial film into the unstrained Si substrate. Except for the Ge and Si layers adjacent to the interfaces, $a_\perp^{s\text{-Ge}}$ is 5.816 Å and $a_\perp^{Si}$ is 5.433 Å. As the thickness of the film is increased from two to ten layers, the value of $a_\perp^{s\text{-Ge/Si}}$ remains constant at 5.630 Å. For the Si and Ge layers adjacent to the interface, the value of $a_\perp^{Si}$ is less by about 0.26% and the value of $a_\perp^{s\text{-Ge}}$ is larger by about 0.29% than their corresponding bulk values. As in the uncapped system the lattice constant of the layers adjacent to the Si/Ge interface can not be predicted by the macroscopic elastic theories.

B. Strained Si in *s*-Si/Ge{001} and Ge/*s*-Si/Ge{001} heterostructures

A similar study has been conducted for the *s*-Si/Ge{001} heterostructure. In this system, the perpendicular lattice constant of the strained Si will be smaller than that of unstrained Si due to the 4.2% increase in the horizontal lattice constant caused by the Ge substrate. Thus, the lattice constant perpendicular to the {001} plane is compressed so as to lessen the increase in strain caused by the expansion of the horizontal lattice constant. Figure 4 contains the same information for the *s*-Si/Ge{001} system that was included in Fig. 2 for the *s*-Ge/Si{001} system. The perpendicular lattice constant, $a_\perp^{Ge}$, for the unstrained Ge substrate is 5.653 Å (shown in layer positions four and five). The perpendicular lattice constant for the bulk-like *s*-Si layers, $a_\perp^{s\text{-Si}}$, is 5.192 Å. The value of $a_\perp^{s\text{-Si/Ge}}$ is 5.444 Å. Elastic theory predicts the perpendicular lattice constant for the bulk-like *s*-Si layers, $a_\perp^{s\text{-Si}}$, to be 5.26 Å, as shown by the dotted line in Fig. 4. This value is higher than that obtained in these simulations. The Si and Ge layers adjacent to the interface again show additional relaxations of 0.004 Å away from and toward the interface, respectively.

The surface reconstructions cause an inward relaxation of 0.27 Å of the topmost *s*-Si layer and an outward relaxation of 0.01 Å of the next inner *s*-Si layer. The inward relaxation of the unstrained silicon (2×1)-dimer reconstructed surface is 0.21 Å. The effect of the surface reconstruction on the strained Si film, which is an increase in the inward relaxation distance from that of the unstrained crystal, is much different from that found for the strained Ge film, which is a decrease in the inward relaxation distance from that of the unstrained crystal. This difference is caused by the compression of the horizontal lattice constant in the strained Ge system as opposed to the expansion of the horizontal lattice constant in the strained Si system. To form a (2×1)-dimer reconstruction, the surface atoms move so that they are close enough to form a bond. This results in a net inward movement of the surface layer. The compression of the horizontal lattice constant in the *s*-Ge system causes the Ge atoms to be closer together than they are in an unstrained Ge crystal; thus, they do not have to move as far inward to be within the Ge dimer bond distance. In the strained Si system, however, the expansion of the horizontal lattice constant from that of an unstrained Si crystal causes the Si atoms to be farther apart; thus, they must move even further inward to be within the Si dimer bond distance. The effects of the surface reconstruction induced relaxations extend five layers deep into the *s*-Si film. They are not, however, as severe as those in the *s*-Ge system. Again these reconstruction induced relaxations are restricted to the epilayers and do not cross the interface into the unstrained Ge substrate, as shown by the curves in Fig. 4 for the two and four layer thick *s*-Si films.

In a recent x-ray photoelectron diffraction (XPD) experiment[4] designed to quantify the strain in a four layer film of Si epitaxially grown on a Ge{001} substrate, the perpendicular lattice constant of the *s*-Si film, $a_\perp^{s\text{-Si}}$, was found to be 5.31($\pm$0.04) Å. The lower limit of this is greater by about 0.07 Å than that of $a_\perp^{s\text{-Si}} = 5.192$ Å, which we found for the bulk-like strained Si layers. As shown in Fig. 4, the perpen-

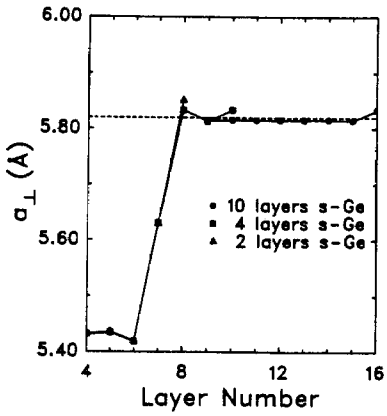

FIG. 3. Same as Fig. 2 except that the *s*-Ge epitaxial layers are sandwiched between two six layer Si films [Fig. 1(b)].

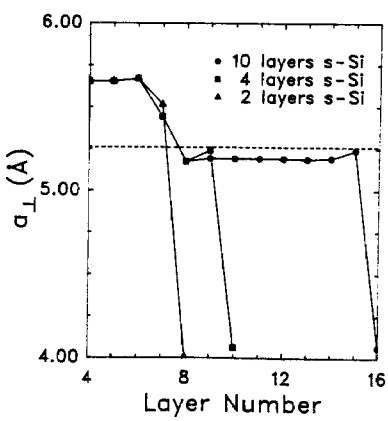

FIG. 4. The variations in the perpendicular lattice constant ($a_\perp$) vs the layer number for a ten layer thick (●), a four layer thick (■), and a two layer thick (▲) strained-Si epitaxial film which has been grown on Ge{001}. The dotted line indicates the *s*-Si lattice constant as predicted by continuum elastic theory.

dicular lattice constant in a four layer strained Si film is not constant. The surface reconstruction induced relaxations cause the perpendicular lattice constant of the first two layers (layer positions nine and ten) to deviate significantly from the bulk value of 5.19 Å. It has been suggested[4] that the averaging effects at the surface, such as the presence of orthogonal (2×1) and (1×2) domains as well as both buckled and nonbuckled surface dimers, will cause the XPD peak to correspond only to the bulk crystal structure. Thus, even though the XPD experiment is performed on a *s*-Si film of only a few layers, it does not address the question of the influence which the surface properties have on the underlying layers of the epitaxial film.

The results of the study of the lattice mismatched strain in the capped Ge/*s*-Si/Ge{001} system are shown in Fig. 5. As in the capped *s*-Ge system, two Si/Ge interfaces exist. The behavior of the *s*-Si about these two interfaces is symmetric, thus in Fig. 5, only the interface between the germanium substrate and the *s*-Si film is shown. The perpendicular lattice constant at the interface, $a_\perp^{s\text{-Si/Ge}}$, is 5.444 Å, while that of the strained-Si film, $a_\perp^{s\text{-Si}}$, is 5.192 Å. These values remain constant as the thickness of the *s*-Si film is increased. Additional relaxations similar to those mentioned above are again seen for the silicon and germanium layers adjacent to the Si/Ge interface.

C. Si_2Ge_2, Si_4Ge_4, Si_3Ge_1, and Si_1Ge_3/Si{001} superlattices

In the Si/Ge heteroepitaxial films studied thus far, the layers adjacent to the interfaces show additional relaxations of the silicon layer away from and of the germanium layer toward the interface. Although these additional relaxations are very small, on the order of 0.30%, they have been shown to affect the electronic structure of Si–Ge superlattices.[20] We have used Tersoff's potential to obtain the fully relaxed geometry of the following four superlattices: Si_2Ge_2/Si{001}, Si_4Ge_4/Si{001}, Si_3Ge_1/Si{001}, and Si_1Ge_3/Si{001}.

In the Si_2Ge_2 superlattice, all of the germanium and silicon atoms are at an interface. Thus, all of the silicon layers should move away from an interface and all of the germanium layers should move toward an interface. The cumulative effect should be an increase of 0.008 Å in the Ge–Ge interlayer distance and a decrease of 0.008 Å in the Si–Si interlayer distance. In an attempt to find whether these changes in the Ge–Ge and Si–Si interlayer distances do exist, we have constructed a twelve layer thick Si_2Ge_2 superlattice supported on a six layer Si{001} substrate. Ignoring the effects of the surface reconstructions, we found the Ge–Ge perpendicular lattice constant, $a_\perp^{Ge}$, to be 5.850 Å and the Si–Si perpendicular lattice constant, $a_\perp^{Si}$, to be 5.403 Å. The perpendicular lattice constant for the Si/Ge interface is 5.630 Å. This geometry is not that used in recent works on the Si_2Ge_2/Si{001} superlattice.[19,21]

In Table I, we compare our perpendicular lattice constants, $a_\perp$, for the epitaxial Si_2Ge_2/Si{001} superlattice with those obtained from elastic theory and LDF calculations,[11] valance force field calculations using *ab initio* force constants,[19] and another empirical potential.[21] The value we calculated for the perpendicular lattice constant of the Si/Ge interface, $a_\perp^{Si/Ge}$, is within 0.07% of that obtained using elastic theory and LDF calculations. The perpendicular lattice constants of the Si and Ge layers, $a_\perp^{Si}$ and $a_\perp^{Ge}$, are 0.032 Å less than and greater than the corresponding values obtained via the elastic theory and LDF calculations.[11] As noted above, this is due to a 0.08 Å relaxation of the Si layer adjacent to the interface away from and of the Ge layer adjacent to the interface toward the interface. Because *ab initio* pseudopotentials generally give smaller equilibrium lattice constants for Si and Ge, the results of the calculations performed using the valance force field method with *ab initio* force constants are in general much smaller than the corresponding results of the other methods. We note, however, that the additional relaxations of the interfacial Si and Ge layers have also been noticed in the *ab initio* force constant method.[19] In Si_2Ge_2, Si_4Ge_4, and Si_6Ge_6 superlattices supported on Si{001} and Ge{001} substrates, they have noticed relaxations of less than 0.005 Å of the Ge layer towards and of the Si layer away from the interface.[19] This is in good agreement with the 0.004 Å relaxation of the interfacial Si layer away from and of the interfacial Ge layer toward the Si/Ge interface found in this work. The other empirical potential method[21] does not show the additional relaxations of the interfacial Si and Ge layers, but instead gives values for the perpendicular lattice constants as would be predicted by simple elastic theory.

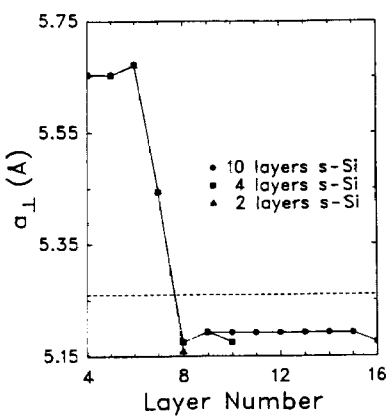

FIG. 5. Same as Fig. 4 except that the *s*-Si epitaxial layers are sandwiched between two six layer Ge films.

TABLE I. Perpendicular lattice constants $a_\perp$ for the epitaxial Si_2Ge_2/Si{001} superlattice.

Work	$^1a_\perp^{Si}$ (Å)	$a_\perp^{Si/Ge}$ (Å)	$^1a_\perp^{Ge}$ (Å)
This work	5.400	5.628	5.852
Elastic theory and LDF calculations (Ref. 11)	5.432	5.624	5.820
Valance force field with *ab initio* force constants (Ref. 19)	5.396	5.572	5.752
Empirical potential (Ref. 21)	5.428	5.612	5.796

The perpendicular lattice constants for Si and Ge, $a_\perp^{Si}$ and $a_\perp^{Ge}$, for this potential[21] are obtained by minimizing the cohesive energy of the superlattice using variationally determined parameters. Thus, a real dynamic relaxation of the lattice is not allowed.

In the Si_4Ge_4 superlattice, not all of the Si and Ge atoms are at an interface. One pair of bulk-like Si and Ge layers exists in each superlattice repeat period. In Table II, we compare our perpendicular lattice constants, $a_\perp$, for the epitaxial Si_4Ge_4/Si{001} superlattice with those obtained via geometry optimized LDF calculations,[20] Keating model calculations,[22] and another empirical potential.[23] In Table II, $^1a_\perp$ refers to the perpendicular lattice constant of a layer adjacent to a Si/Ge interface, and $^2a_\perp$ refers to the interplanar distance of a bulk-like layer. At the Si/Ge interface, we find additional relaxations of the adjacent Ge layer toward the interface and of adjacent Si layer away from the interface. These types of additional relaxations have also been seen in the recent geometry optimized LDF calculations of Ciraci and Batra.[20] The qualitative trends in the values of the perpendicular lattice constant in Si layers, Si/Ge interface and in Ge layers as obtained in our calculations are the same as those of Ciraci and Batra.[20] Their values for the perpendicular lattice constants, however, are consistently smaller than our values. This again is because *ab initio* pseudopotentials generally give smaller equilibrium lattice constants for Si and Ge. Our results agree quite well with those obtained via the Keating model calculations.[22] They find the same trend in the relaxations of the interfacial Si and Ge layers as obtained in our work. We note, however, that the parameterization for the Keating model calculations[22] has to be readjusted whenever a new superlattice or a thin film geometry is encountered. We, on the other hand, have obtained reasonably good equilibrium geometries of many different epitaxial films and superlattices configurations without making any adjustment to Tersoff's potential.[12] The calculations done with the other empirical potential[23] do not show the additional relaxations of the interfacial layers. The potential used in these simulations[23] is an expanded version of the Stillinger–Weber potential which has been fit to both Si, Ge, and SiGe. It was optimized for the melting properties of Si and not for the elastic properties of Si or Ge. This could account for why it does not show the additional relaxations of the interfacial layers as seen in both the LDF calculations and in our work using Tersoff's potential. Also this potential gives a much larger Ge perpendicular lattice constant, $a_\perp^{Ge}$, than found by any of the other methods. This may be due to the manner in which the potential was expanded to describe Ge.

TABLE III. Perpendicular lattice constants $a_\perp$ for the epitaxial Si_3Ge_1/Si{001} and Si_1Ge_3/Si{001} superlattices.

Superlattice	$^1a_\perp^{Si}$ (Å)	$a_\perp^{Si/Ge}$ (Å)	$^1a_\perp^{Ge}$ (Å)
Si_3Ge_1	5.420	5.648	···
Si_1Ge_3	···	5.616	5.832

The fully relaxed geometries of the Si_3Ge_1 and Si_1Ge_3 superlattices have also been calculated. Table III contains the values of the perpendicular lattice constants found for these fully relaxed superlattices. In the Si_3Ge_1 superlattice, no Ge–Ge perpendicular lattice constant has been calculated since each germanium layer is sandwiched between two silicon layers; thus only values for $^1a_\perp^{Si}$ and $a_\perp^{Si/Ge}$ can be calculated. In the Si_1Ge_3 superlattice, only values for $a_\perp^{Si/Ge}$ and $^1a_\perp^{Ge}$ have been calculated since no Si–Si interlayer spacings exist because each silicon layer (disregarding those in the substrate) is sandwiched between two germanium layers. The perpendicular lattice constant for the Si/Ge interface in the Si_3Ge_1 superlattice is 0.33% greater than and that for the Si_1Ge_3 superlattice is 0.23% less than the corresponding values for the Si_2Ge_2 and Si_4Ge_4 superlattices. Since in the Si_3Ge_1 superlattice, the silicon layers sandwiching the germanium layer are both moving away from the germanium layer, the Si/Ge interlayer spacing increases; and thus, the Si/Ge perpendicular lattice constant increases. In the Si_1Ge_3 superlattice, the germanium layers are moving toward the silicon layer so the Si/Ge perpendicular lattice constant decreases. To our knowledge, these are the first calculations of the fully relaxed geometries of the Si_3Ge_1/Si{001} and Si_1Ge_3/Si{001} superlattices.

IV. DISCUSSION

In summary, we have addressed the quantification of uniaxial strain in Si/Ge heteroepitaxial films and superlattices via Tersoff's many-body potential and the quasi-dynamic

TABLE II. Perpendicular lattice constants $a_\perp$ for the epitaxial Si_4Ge_4/Si{001} superlattice.

Work	$^2a_\perp^{Si}$ (Å)	$^1a_\perp^{Si}$ (Å)	$a_\perp^{Si/Ge}$ (Å)	$^1a_\perp^{Ge}$ (Å)	$^2a_\perp^{Ge}$ (Å)
This work	5.432	5.416	5.632	5.832	5.812
Geometry optimized LDF calculations (Ref. 20)	5.420	5.388	5.564	5.716	5.700
Keating model calculations (Ref. 22)	5.432	5.424	5.632	5.868	5.832
Empirical potential (Ref. 23)	5.428	5.428	5.596	5.964	5.964

method. Although the size of our films approaches the accepted critical thickness for Si/Ge epitaxial growth, we do not find any indications of defect formations in our simulations. The strains calculated for the bulk-like Si and Ge layers and for the Si/Ge interface embedded in bulk agree well with those predicted by macroscopic elastic theory.[11] At the Si/Ge interface, we find that the adjacent Ge layer relaxes towards the interface and that the adjacent Si layer relaxes away from the interface. The magnitude of these additional relaxations are in agreement with those of the recently published geometry optimized LDF calculations.[13,20] Since these relaxations are not affected by the thickness of the film or by which component, Si or Ge, is strained, it appears as if this is a chemical and not just a physical phenomena.

In the uncapped strained epitaxial films, the effects which the surface reconstructions have on the top layers of the epitaxial film are studied in detail. We find that a (2×1) dimer reconstruction of the surface layer significantly alters the strain values of the top five epilayers. If the epitaxial film is less than five layers thick, the effects of the surface reconstruction are restricted to the epitaxial film and do not cross the interface into the substrate. We find that the inward relaxation of the reconstructed surface layer on a strained Si or Ge film is different from that on the unstrained Si or Ge film. The reconstructed surface layer of the *s*-Ge film has a much smaller inward relaxation than the reconstructed surface layer of the *s*-Si film. This is because in the *s*-Ge film, the surface reconstruction induced relaxations are in the opposite direction to the relaxations caused by the lattice mismatched strain; whereas, in the *s*-Si film they are in the same direction as the relaxations caused by the lattice mismatched strain. The calculated strains of 5.192 Å in the bulk-like *s*-Si layers and of 5.816 Å in the bulk-like *s*-Ge layers are in good agreement with the available experimental results of $a_{\parallel}^{s\text{-Si}} = 5.31$ Å[4] and $a_{\parallel}^{s\text{-Ge}} = 5.84$.[9] The experiments, however, are only sensitive to the measurement of the strain in the bulk *s*-Si and *s*-Ge layers and not the surface layer.[4] In addition to the quantification of the strain in the bulk-like *s*-Si and *s*-Ge layers, our calculations also provide a quantitative look at how the surface reconstructions influence the relaxation of the strained layers in the underlying thin epitaxial film. These values will be useful for electronic band structure calculations of thin heteroepitaxial films of *s*-Si and *s*-Ge layers.

The fully relaxed geometries of the Si_2Ge_2/Si{001}, Si_4Ge_4/Si{001}, Si_3Ge_1/Si{001}, and Si_1Ge_3/Si{001} superlattices are also obtained. The trends seen in the strain values of Si_4Ge_4/Si{001} superlattice are in good agreement with those obtained by the geometry optimized LDF calculations.[20] The results of calculations done using two other empirical potentials[21,23]; Khor's and Das Sarma's empirical potential[21] for the Si_2Ge_2/Si{001} superlattice and an expanded Stillinger–Weber potential[23] for the Si_4Ge_4/Si{001} superlattice, do not show the additional relaxations of the interfacial layers as seen in the geometry optimized *ab initio* calculations[13,20] and in our work using Tersoff's potential.[12] Thus, Tersoff's potential has been found suitable for studying the strain in Si/Ge heterostructures and superlattices.

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