Elasticity-based theory of misfit-induced structural defects at semiconductor interfaces

P. Masri
Groupe d'Etude des Semiconducteurs, URA 357 du Centre National de la Recherche Scientifique, Université Montpellier 2, Sciences et Techniques du Languedoc, Place Eugène Bataillon, 34095 Montpellier Cédex 5, France
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In this paper, we consider the problem of the determination of misfit-induced structural features at the interface of semiconductor heterostructures. We then develop a theory which enables us to investigate these features. This theory is based on the elasticity equations within the range of application of Hooke's law. The main aim of the theory is the determination of the parameter n_s which defines the superstructure which may stabilize the interface between the host materials constituting the heterostructure. This is done by identifying, in the elasticity equations, the S factor, i.e., $S=C_{ij}/\rho$, as the important parameter which must be considered within an approach which takes account not only of the mismatch of the lattice parameters of the host materials, but also of the difference in elastic-density features. The periodic sites of the defined super unit cell, induced by the misfit, may be considered as nucleation centers for misfit-dislocations network. Due to the lattice misfit, one must seek an optimized choice of the materials and of the growth conditions. In heterostructures where a large misfit exists, the insertion of a transitional layer aiming to obtain high-quality heterostructures may often be useful. We demonstrate that the present theory may be used to predict the composition of such transitional layers.

I. INTRODUCTION

Modern crystal-growth techniques can now afford a wide panoply of artificially made heterosystems for applied physics purposes. To be efficient, these techniques must be based on a comprehensive understanding of the physics involved in the field of crystal growth. We deal here with problems involving the macroscopic and microscopic aspects of interface physics. The macrophysics (macrointerface) aspect of heteroepitaxy must be taken into account because not only local characteristics but also periodic and long-range features influence the process. This is, for example, the case of Lomer dislocations which may be created at the interface between two host materials with mismatched lattice parameters when, for example, the layer thickness exceeds a critical value: in GaSb/GaAs heterostructures, these edge dislocations have been observed as a periodic square array of dislocation network localized near the interface. In this system,[1] the associated dislocation spacing is equal to 56 Å when one applies only geometric considerations and assumes that 100% of the misfit is accommodated by misfit dislocations (MD's). As we know, these structural defects are associated with misfit strains induced by the lattice-parameter mismatch. An energy balance between strain-associated elastic energy and dislocation formation energy determines the overlayer critical thickness beyond which MD's are energetically more favored than strains.

Clearly speaking, the periodicity of the MD network (the superunit cell associated with these defects) is the important parameter which determines the dislocation density and, consequently, because of the energy balance which triggers the MD regime, the overlayer critical thickness. It then appears that it is essential to consider a proper description of the MD network. In Sec. II, we present the theory which enables to carry out such a program. We then apply it to different heterostructures.

II. S-CORRELATED THEORY OF MISFIT-INDUCED SUPERSTRUCTURES

It is our claim that, to reach this aim, one must incorporate in the theory not only geometric factors such as the lattice parameter mismatch but also mismatched elastic features. To do so, a good starting point is to build up a theory based on the interaction of the elastic fields which arise from and act on the host materials in the considered heterostructure. These elastic fields are generally well described by using Hooke's law which is valid in the range of small strains: this law states that, in an elastic solid, the strain is proportional to the stress. The strains we are interested in are those induced by the mismatch of the lattice parameters of a substrate material (A) and an overlayer (B). Within this approximation, our theoretical approach must indeed be based on the equations of elasticity as stated, for example, for cubic crystals:[2]

$$\frac{\delta^2 u}{\delta t^2}=\frac{C_{11}}{\rho}\frac{\delta e_{xx}}{\delta x}+\frac{C_{12}}{\rho}\left[\frac{\delta e_{yy}}{\delta x}+\frac{\delta e_{zz}}{\delta x}\right]+\frac{C_{44}}{\rho}\left[\frac{\delta e_{xy}}{\delta y}+\frac{\delta e_{zx}}{\delta z}\right], \tag{1}$$

In Eq. (1), u is the x component of the displacement, ρ is the density, C_{ij} are the elastic constants, and $e_{\sigma\sigma'}$ are the strain components ($\sigma,\sigma'=x$, y, or z). The equations for the directions y and z can be deduced from Eq. (1). The resulting equations may be considered as the signature of strain-induced lattice dynamics, correlated via the S factor ($S=C_{ij}/\rho$). The left-hand side of Eq. (1) is propor-

tional to ω^2, the square of the angular frequency ω.

The most striking feature of semiconductor surfaces is that they may undergo a wide variety of surface reconstructions as they are subjected to external forces and strain-induced elastic fields due to adsorption or segregation processes. The current development of surface technology enables us to provide reliable evidence of the resulting superstructures, as for example the 7×7 reconstruction of the Si(111) surface observed with the scanning-tunneling-microscopy technique. The physics involved in modern growth processes must deal with surface problems, as the initial surface arrangement of the substrate may determine the initial stages of the growth process. Many studies have recognized the role of strain in taking up the lattice mismatch between the reconstructed surface layer and the inner part of the crystal. We are interested here in the interface problem addressed by modern growth experiments, where heterostructures, constituted of materials having different lattice parameters, are made. Again, the role of strain has been identified as an important mechanism in the stabilization of interfacial structural features.

Let us represent by $(m\times n)a$ the size of a unit cell which may stabilize the surface of a semiconductor subject to different interactions; here a represents the lattice parameter, and m and n are the integers which define the in-plane (x,y) periodicity of the superstructure. The periodic conditions allow a Fourier analysis of all equations and parameters. This leads to the concept of the two-dimensional Brillouin-zone representation (2DBZ) of the dynamical waves and their frequencies: this is based on the quantification of the phonon wave vector. The extensions of this 2DBZ along x and y, respectively, are equal to $g_x\approx\pi/ma$ and $g_y\approx\pi/na$. We can eventually deduce from Eq. (1) and from the above analysis that the phonon frequencies clearly depend on the S factor and on the geometric factor $G\equiv1/g_xg_y\propto(m\times n)a^2$, as $\omega^2\propto SG^{-1}$. A phonon-frequency matching relationship between materials A and B leads to the equation

$$G_BG_A^{-1}=S_BS_A^{-1}\ , \tag{2}$$

where

$$S_{A,B}=(C_{11}/\rho)_{A,B} \tag{3}$$

and

$$G_A\propto(p\times q)a_A^2\ , \tag{4}$$

$$G_B\propto(m\times n)a_B^2\ . \tag{5}$$

G_A and G_B are the geometric factors of the substrate and of the overlayer, respectively; a_A and a_B are the corresponding lattice parameters; and the integers p and q scale the surface superstructure of the substrate prior to overlayer deposition.

Equation (2) represents the condition which must be fulfilled by substrate and overlayer features when we take account of the mismatch of the S factors of the host materials, i.e., $S_A\neq S_B$. It correlates geometric and S factors to predict the stable superstructure (G_B) which may exist at the A/B interface. Such a correlation relates G_B, the final interface structure accommodated by A and B, to that (G_A) of the substrate initial surface structure via the S factor. This correlation has been successfully applied to several systems[3,4] such as SiO_2(coesite)/Si, Ge/Si, a-Si/$Ge_{0.2}Si_{0.8}$, and $Ge_{0.5}Si_{0.5}$/Si and has allowed us to predict,[5] for Si_xGe_{1-x}/Si interfaces, the evolution of the interface superstructure with the Si composition x.

At a nanometric scale, the lattice misfit involves the difference $|a_A-a_B|$. Associated with this quantity, we may define a "small" Burgers vector $b_e=a_B-a_A$, with $a_B>a_A$. In the case of perfect epitaxy, this corresponds to small epitaxial dislocations: b_e represents a rather small fraction of the lattice parameters. By a vernier effect, we end up with a network of epitaxial MD's which are fairly parallel and more or less equidistant to each other, with a lattice spacing equal to L. If $b_e\to0$, one may expect that $L\to\infty$. The appearance of the MD's corresponds to a negative free energy associated with these defects, as they aim to relax the interface strains. Let us assume that we apply isotropic conditions in the interface plane, so that $m=n$ and $p=q$, and the MD network is a square lattice along x and y directions. To ensure a lattice matching between the host materials constituting the heterostructure, we must look for stable interface superstructures which may depend not only on geometric features but also on the S factor as derived from the elasticity equations of dynamics. Dynamics is involved here because strain-induced reconstruction processes imply atomic displacements. In this way, we can define a periodic interface geometry where nucleation centers for MD's (MDNC) may be created, resulting in a network of parallel MD of separation L. L is usually determined by the following geometric condition:[6]

$$(n_1+1)a_A=n_1a_B\quad\text{if } a_A<a_B\ . \tag{6}$$

We then obtain

$$n_1=a_A/(a_B-a_A)\ . \tag{7}$$

Equation (6) implies that after n_1 jumps on the lattice under compression (here B) and (n_1+1) jumps on the lattice under extension (here A), we obtain a coincidence of the two lattices. Knowing n_1, we can calculate the lattice spacing L of MD's.

Considering now a comprehensive approach of the heteroepitaxy problem, and not only geometric requirements, we may find the interface geometry which accommodates the lattices A and B by using the correlation theory of misfit-induced superstructures (MIS's). To do so, we introduce a superstructure parameter n_s, and express the geometric factors G_A and G_B in function of n_S as

$$G_A\propto(n_S+1)^2a_A^2\ , \tag{8}$$

$$G_B\propto n_S^2a_B^2\quad\text{with } a_B>a_A\ . \tag{9}$$

Equations (2)–(5) and (8) and (9) give the relationship

$$(n_S+1)a_A=a_Bn_S/\sqrt{S}\quad\text{with } a_B>a_A \tag{10}$$

where

$$S = S_B / S_A \ . \tag{11}$$

By analogy with Eq. (6), Eq. (10), which gives n_S, represents the S-factor-correlated theory of MIS's and of the related structural features of the MD network confined to the A/B interface. Equation (10) gives

$$n_S = a_A (a_B \sqrt{S} - a_A)^{-1} \ . \tag{12}$$

If $S=1$, one can see that $n_S = n_1$: this means that we may obtain an interface geometry which gives an amount of MDNC's comparable with that predicted by Eq. (6) only if the condition of S-factor matching is fulfilled. If material A is under compression, and B is under extension ($a_A > a_B$), we obtain

$$n_1 a_A = (n_1 + 1) a_B \tag{13}$$

and

$$n_1 = a_B / (a_A - a_B) \tag{14}$$

for the geometric theory, and

$$n_S = a_B / (a_A \sqrt{S} - a_B) \tag{15}$$

for the present S-factor-correlated theory of MIS and MD networks. If we keep unmatched the S factors, n_S is smaller than n_1. This means that with the structural configuration n_S, precursor to the creation of the MD network, the lattice spacing L predicted by the present theory is smaller than that obtained with Eqs. (6) and (13) which correspond to a quasiperfect strain relaxation.

III. APPLICATION TO DIFFERENT HETEROSTRUCTURES

In what follows, we apply the S-factor-correlated theory to a wide variety of heterostructures in order to demonstrate the general trends of our approach. Then we discuss in detail some particular systems.

A. General trends

In Fig. 1 we represent the variation of n_S as a function of S for different heterostructures. In all cases, we calculate the geometric and S factors by using the bulk parameters. One can see that the highest values of n_S, i.e., the smallest amounts of MDNC's, are obtained for $S \cong 1$, and that n_S decreases when the mismatch of the S factors increases. Outside the range of matching of S ($S \neq 1$), $n_S < n_1$ and, consequently, we expect an enhanced amount of MDNC's. Two parameters are relevant to the n_S values, namely the S factor and the misfit f defined by the relationship[7]

$$f = 2(a_B - a_A)(a_A + a_B)^{-1} \ . \tag{16}$$

A small amount of MD centers is indeed obtained for heterostructures with a good matching of the S factors and small misfit f.

Among all investigated systems, it is the InAs/GaSb heterostructure which has the highest value of n_S, then followed by $C_{0.02}Si_{0.98}$/Si. These systems are characterized by small values of the misfit f and an S factor close to 1.

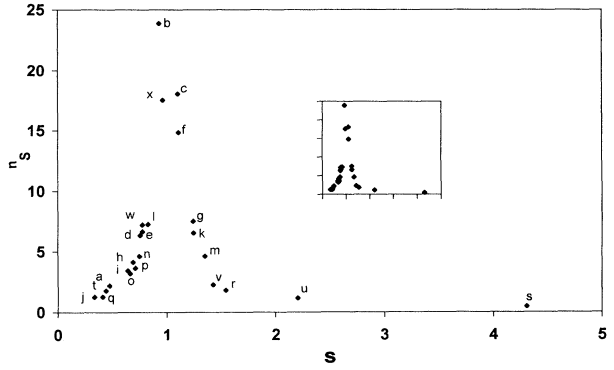

FIG. 1. Variation of the MIS parameter n_S as a function of the S factor for different heterostructures. The inset gives a view of the shape of the curve and shows the peak near $S=1$. (a) GaP/Si. (b) InAs/GaSb. (c) $C_{0.02}Si_{0.98}$/Si. (d) $Si_{0.8}Ge_{0.2}$/Si. (e) $In_{0.74}Ga_{0.26}As$/InP. (f) $In_{0.8}Ga_{0.2}P$/InP. (g) $GaAs_{0.5}P_{0.5}$/GaAs. (h) InAs/InP. (i) GaAs/GaP. (j) Ge/Si. (k) $In_{0.5}Ga_{0.5}As$/InP. (l) $In_{0.5}Ga_{0.5}As$/GaAs. (m) $In_{0.3}Ga_{0.7}As$/InAs. (n) $In_{0.74}Ga_{0.26}As$/GaAs. (o) InAs/GaAs. (p) GaSb/GaAs. (q) CdTe/GaAs. (r) β-SiC/Si. (s) C/Si. (t) GaN/β-SiC. (u) GaN/GaAs. (v) GaN/GaP. (w) ZnSe/GaAs. (x) InP/GaAs.

In Fig. 2, we represent the variation of n_S in function of the misfit f. One can see that n_S decreases when f increases, and these variations are weighted by S. The effect of S is very sensitive for GaP/Si which presents a small misfit but a large S mismatch. This gives a small value of n_S and eventually corresponds to a system where an enhanced amount of MDNC may be created. These results for n_S may be compared with those represented in Fig. 3 showing the variation of n_1 as a function of f. One can deduce that the geometric conditions, i.e., Eqs. (6) and (13), lead to values of n_1 higher than n_S, as these equations apply for $S=1$. This latter S-factor-matching condition may then appear as having a stabilizing effect on the interface,[8] and as a factor of interface quality, because of the small amount of predicted extended defects

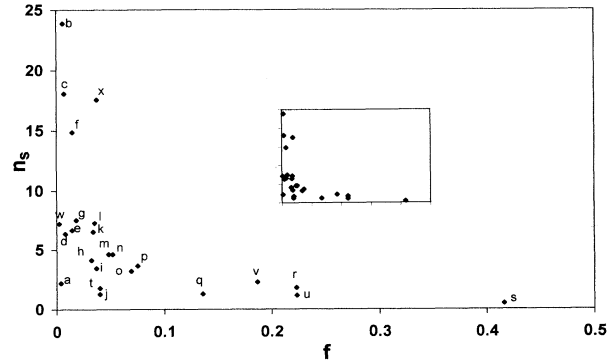

FIG. 2. Variation of the MIS parameter n_S as a function of the misfit for different heterostructures. The inset gives a view of the shape of the curve. (a)–(x) are the same as in Fig. 1.

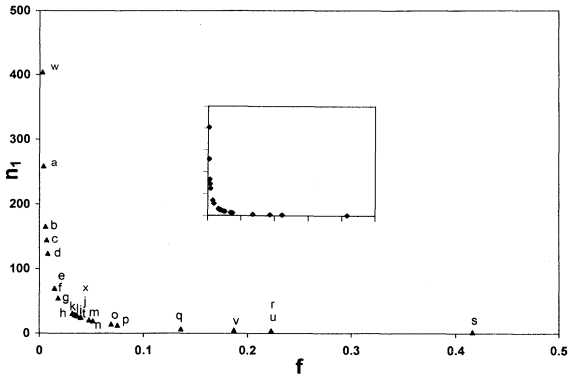

FIG. 3. Variation of the MIS parameter n_1 calculated by using the geometric theory (Ref. 6). The inset gives a view of the shape of the curve. (a)–(x) are the same as in Fig. 1.

when it becomes fulfilled. For ZnSe/GaAs, the condition $S=1$ leads to a giant MIS of the MD network as $n_1 \cong 404$, while the present theory, by taking account of the mismatch of the S factors ($S \cong 0.78$), gives $n_S \cong 7$. This represents a huge difference, and we emphasize the strong sensitivity of the size of the unit cell of the MD network to the S factor as it is present in the elasticity theory. Obviously, one cannot circumvent the reality of the S-factor mismatch and its implications for the structural features of the MD network, as the consideration of such a parameter is a natural consequence of the application of the elasticity theory. From this point of view, it is our claim that the geometric features of the MD network must be related, somehow, to S: the creation of MD's is indeed triggered by an energy-balance mechanism which involves the energy associated with elastic strain due to lattice mismatch and that necessary to create a MD network. However, if the values of n_1 may seem too large for some systems, the values of n_S may also appear to be too small, leading to a high density of MD's. One can then imagine that, as the growth process is going on, and near the transition from the regime of elastic strain toward the dislocation regime which relieves these strains, a matching of the S factors may take place.

The present theory states that, for large misfit, n_S becomes small and of an order of magnitude comparable to n_1. This is, for example, the case for InAs/GaAs, GaSb/GaAs, CdTe/GaAs, β-SiC/Si, GaN/GaP, GaN/GaAs, and C/Si (see Figs. 2 and 3). The present theory tells us that if, in these heterostructures, we incorporate, at the early stages of the growth process, a mechanism which may improve the matching of the S factors near the interface, this will increase n_S and, consequently, decrease the amount of MDNC's. Such mechanisms must, in particular, result in a softening or stiffening of the elastic properties of the host materials near the interface. They may be based on (i) surface and extended defects creation, (ii) impurity incorporation, (iii) temperature effects if the temperature coefficients of the thermal expansion of host materials are very different, or (iv) alloying effects.

In terms of the amount of MDNC's, the advantage presented by the condition of matching the S factors of a given heterostructure, in improving the interface stability, is shown by the results presented in Fig. 1.

B. Case of InP/GaAs heterostructure

If we consider systems such as InP/GaAs, Ge/Si, GaAs/GaP, GaN/β-SiC, and $In_{0.5}Ga_{0.5}As$/GaAs, they are all characterized by nearly the same value of the misfit f. However, their S factors are different (see Fig. 1), and among all these systems it is the InP/GaAs one which presents the best matching of the S factors ($S \cong 0.96$). Consequently, this latter heterostructure has the largest value of n_S, i.e., the smallest amount of MDNC's as predicted by the S-factor-correlated theory of the MD network. Such a heterostructure has been suggested to fabricate a laser.[9] It has recently been grown by low-pressure metal-organic vapor-phase epitaxy.[10] In order to reduce the dislocation density, different methods have been proposed. They consist in inserting (i) strained-layer superlattices[11] (SLS's) or (ii) a single strained interlayer (SIL) of $In_{1-x}Ga_xP$.[10] The optimization of the properties of the SIL has shown that $x \cong 0.2$ corresponds to a good choice. The effect of $In_{0.33}Ga_{0.67}As$ and $In_{0.74}Ga_{0.26}As$ SIL's has been investigated[10] and compared to that of $In_{0.8}Ga_{0.2}P$. After insertion of the SIL, we must deal with a two-interface system, namely SIL/InP and InP/GaAs. The discussion concentrated on the reduction of the amount of MDNC's in the InP layer due to the intercalation of the SIL. The interpretation of the experimental results has led to the following conclusions: for the $In_{0.74}Ga_{0.26}As$ SIL, interface MD's may be not arranged as a network, and this is explained as due to the compressive strain in the SIL. For the $In_{0.33}Ga_{0.67}As$ SIL, the conclusion was that remnant strain is less than in the $In_{0.8}Ga_{0.2}P$ SIL and that, in the former layer, strains are more easily relaxed than in the latter layer. On the whole, these results cannot be well understood within the framework of the only geometric approach [Eqs. (6) and (13)]. Figure 3 shows indeed that the three SIL's studied in Ref. 10 give a value of n_1 (i.e., a value of dislocation spacing) higher than that obtained for the InP/GaAs interface. It is then hard to understand why the MD's will be preferentially attracted by the interfaces introduced by the former three SIL's, even if a smaller MD density (higher n_1) is expected. On the contrary, the present S-correlated theory of MDNC's predicts smaller values of n_S (i.e., higher MD densities) for the $In_{0.8}Ga_{0.2}P$ and the $In_{0.74}Ga_{0.26}As$ SIL's than for the InP/GaAs interface. Moreover, our results suggest that the $In_{0.8}Ga_{0.2}P$ SIL gives a MD network unit cell (n_S) close to that of the InP/GaAs interface, in agreement with the experimental optimal conditions defined in Ref. 10. This SIL choice ensures a geometric continuity when we move from the InP/GaAs interface toward the $In_{0.8}Ga_{0.2}P$/InP interface. This is not the case for the $In_{0.74}Ga_{0.26}As$ SIL, as it corresponds to a value of n_S much smaller than that associated with the InP/GaAs system. The present theory tells us that we may also

reach a better structural continuity between the two interfaces if we use a SIL with an In concentration equal to 83%: in this case, the $In_{0.83}Ga_{0.17}P/InP$ interface is stabilized by a superstructure corresponding to $n_S \cong 18$, exactly the same superstructure which stabilizes the InP/GaAs interface.

C. Case of GaSb/GaAs heterostructure

Let us now consider the GaSb/GaAs heterostructure. This represents a promising material for optical applications. The optimization of the heterostructure features aimed to produce systems with low dislocation density and a fairly good photoluminescence spectra, despite the high lattice misfit, which is about 7.5% in this system. To realize such a project, thin epilayers of GaSb have been grown by using modern growth techniques such as metal-organic vapor-phase epitaxy[12] (MOVPE) or molecular-beam epitaxy[13,14] (MBE). Beside all the available techniques for the optimization of the interface quality (insertion of SLS's or SIL), one may also consider the growth of a transitional layer of $GaAs_{1-x}Sb_x$ in order to minimize the lattice mismatch which exists between GaSb and GaAs. The growth of such alloy epilayer on GaAs(100) has been carried out by MBE.[13,15,16] Although a miscibility gap may exist for the alloy $GaAs_{1-x}Sb_x$, and depending on the growth technique used, the growth of this alloy may be achieved over the entire composition range with a single-crystal phase for all the grown layers.[15,16] In Ref. 16, it has been shown that the fundamental physics, involved in the growth process at an atomic scale (e.g., interface reconstruction), may be correlated with the lattice mismatch which depends on the relative composition of Sb and As: for $x \geq 0.8$, it has been observed that surface reconstruction of the alloy are analogous to those of GaSb, whereas they are analogous to those of GaAs for $x \leq 0.5$. This means that, in the intermediate range of x, there exists an optimized choice of the transitional layer composition which is suitable to obtain high-quality heterostructures. In what follows, we apply the S-correlated theory of MIS's to the GaSb/GaAs interface, and we demonstrate that our approach may be useful to make such an optimized choice, and that the theoretical issue corresponds to a realistic situation which makes contact with experimental results with respect to two aspects: (i) the fabrication aspect which is aimed by determining the alloy composition, and (ii) the growth physics aspect on an atomic scale; this latter involves the structural configuration of the interface and its consequences on the geometric features of misfit-induced extended defects.

The ultimate chemical state of the heterostructure we consider here is the GaSb/GaAs system, with a misfit equal to 7.5%. This is the limit $x = 1$ for Sb composition. However, we may reduce this misfit by varying x ($x < 1$), i.e., by increasing the As composition of the alloy layer. The system we consider here is the one where the alloy layer plays the role of a transitional layer (buffer layer) on the top of which the growth of the GaSb layer will eventually take place. We then must consider two heterointerfaces, namely the $GaAs_{1-x}Sb_x/GaAs$ interface (interface 1) and the $GaAs_{1-x}Sb_x/GaAs$ interface (interface 2). Each of them is characterized by an S factor (respectively S_1 and S_2), and we define an average value of S as $S_{av} = 0.5(S_1 + S_2)$. The idea which is behind the introduction of such an average value for the transitional layer is that we may consider this latter as a reference interface for GaSb and GaAs: it is aimed at ensuring a continuity, through the heterostructure, of features relevant to the problem we consider: continuity for geometric properties and for other elastic properties as present in the elasticity theory. The occurrence of such a transitional layer may be a realistic situation: after all, we know that interfacial mixing may be an inherent process in interface physics.

In what follows, we use bulk parameters for all three materials, namely GaSb, $GaAs_{1-x}Sb_x$ and GaAs; we assume, as has been demonstrated in Ref. 15, that the Vegard law is satisfied over in nearly the entire range of x. We represent in Fig. 4 the spatial periodicity (L) of MIS's for interfaces 1 and 2 and, as discussed, this may represent the lattice spacing of a precursor state for the MDNC network: curves 1 and 2 represent the results of the geometric[6] approach [Eqs. (6) or (13)], while curves 3 and 4 give results obtained with the S-correlated theory. The results demonstrate that indeed there exist a Sb composition for which the superstructure periodicities associated with interfaces 1 and 2 are the same: this is shown by the crossing of curves 1 and 2 for the geometric approach, and that of curves 3 and 4 for the S-correlated theory. In this latter case, the crossing occurs at $x \cong 0.53$: this corresponds to a periodicity equal to 34 Å. In the former case, the crossing occurs at $x \cong 0.48$ with a periodicity equal to 110 Å. We must recall that, in our approach, we use bulk parameters to calculate this interface periodicity which fits both interfaces, and that, unfortunately, we know the little about the values of, e.g., elastic properties when and where MD's may develop subsequently to strain relief. If we assume that, during the growth process, a matching of the elastic features may take place, triggered by a mechanism of minimiza-

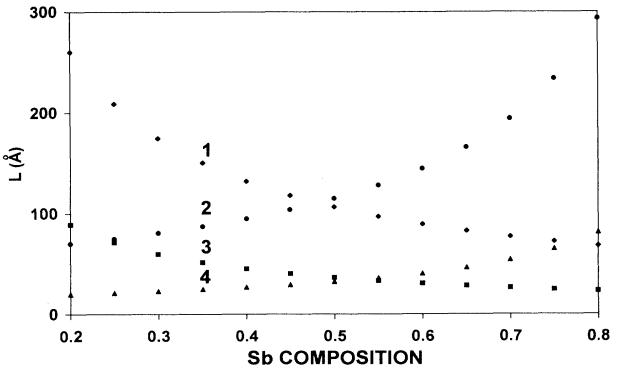

FIG. 4. Variation of the spatial periodicity of the MIS's associated with the GaSb/GaAs heterostructure in function of the Sb composition of the $GaAs_{1-x}Sb_x$ transitional layer: curves 1 and 2, respectively, represent the results obtained with the geometric theory (Ref. 6) for the interfaces $GaAs_{1-x}Sb_x/GaAs$ and $GaAs_{1-x}Sb_x/GaSb$. Curves 3 and 4 correspond to the results obtained with the S-correlated theory of MIS.

tion of the interfacial energy, this will result in an adjustment of the S factors of the host materials ($S \cong 1$). In this way, the values of the superstructure periodicity predicted by the present theory shift to higher values comparable to those given by the geometric approach.[6]

However, beyond this hypothetical point of view about a possible mechanism for S-factor matching, a straightforward strategy would be to make an optimized choice of the composition of the transitional layer which may ensure such a matching of S. In what follows, we demonstrate that such a strategy is possible with our approach. In order to establish the relevance of S for growth physics, we represent in Fig. 5 the values of S_{av} as a function of the Sb composition x. We discover that $S_{av} \cong 1$ for $x \cong 0.57$. This corresponds to a transitional layer of composition $GaAs_{0.43}Sb_{0.57}$. This value of x is very close to that ($x \cong 0.53$) which corresponds to the geometric matching of the two interfaces. In Ref. 15, by using the continuously grading technique of growth, a layer of composition $GaAs_{0.42}Sb_{0.58}$ has been grown, by using the molecular-beam epitaxy technique, with a continuously grading buffer layer on a GaAs(001) substrate. This had led to the preparation of high-quality $GaAs_{1-x}Sb_x$ layers corresponding to this latter experimentally aimed composition. Thus the composition of the transitional layer predicted by the S-correlated theory of MIS's corresponds to a realistic and valuable choice which was experimentally selected several years ago. It is now within the present theory that we may better understand the physics underlying such a choice, and why it is an optimized one: this requires not only a geometric matching of the interfaces between the transitional layer and its surrounding, but also a matching of the associated S factor. Through the application of the continuity conditions, we may consider that the introduction of such a transitional layer is one possible mechanism contributing to the stability and the high quality of interfaces.

IV. CONCLUSION

We have presented a theory of MIS's in semiconductor heterostructures based on the elasticity theory. Our approach resumes with the obtaining of continuity conditions for geometric and elastic-density features of interfaces formed between the host materials constituting the system. These continuity conditions enable us to make optimized choices in building up the heterostructure. Our starting point is formulated within the framework of the correlation theory[3–5] which, applied to several heterostructures, has successfully predicted their stable interface structure. We are then able to determine, for each heterointerface, a MIS defined by n_S, which fits the interface lattices of the host materials in contact.

The misfit which exists between two materials constituting a heterostructure may be taken up by interface strains as long as the layer thickness does not exceed a critical value h_c. Beyond h_c, the creation of MD's is observed as a mechanism which may relieve these misfit strains. We may also learn from thermodynamics that, for $h > h_c$, the cost in energy E_d in relieving the strains by creation of MD's is smaller than E_S, the elastic energy in strained heterostructures. For many heterosystems, these MD's may exist as a network of parallel dislocations with a periodicity defined by their lattice spacing L. We may then consider the MIS obtained within our approach as a precursor configuration defining a periodic distribution of MDNC's where MD's may be eventually created. Our approach involves not only geometric factors, as stated by the usual theory[6] predicting the lattice spacing L of the MD network, but also elastic-density factors ($S = C_{ij}/\rho$) as present in the elasticity theory. This approach is the S-correlated theory of MIS's. It is equivalent to the geometric approach[6] for $S = 1$.

During the growth process, when the experimental conditions are suitable for a transition from the elastic strain regime toward the MD regime, among all the questions which must be raised, two are relevant to our approach: (i) What is going on for the geometric mismatch? (ii) How can the S-factor's possible modification be incorporated into the process? This latter effect is important to consider because it introduces, in the energy balance between elastic strains and MD's, a specific contribution which certainly must affect the effective values of overlayer critical thicknesses. The MIS parameter n_S which we calculate can be considered, in this transition regime, as representing a structural state precursor to the creation of MDNC's. Although we know little about the behavior of elastic, density, and geometric parameters just before and during the transition regime, we have simulated the dependence of n_S on the misfit and on S by using the bulk values of the involved parameters. We discover that, in agreement with interface stability requirements, the curve $n_S(S)$ shows a maximum near $S = 1$, where one can expect low values of MD density. For a given heterostructure built up without any trick in order to optimize the interface quality, this matching of the S factors of the constituting host materials may or may not be fulfilled. However, its application represents an advantage which can be expressed in terms of system optimization. This strategy leads to obtaining continuity conditions which apply, through the heterostructure, to microscopic features such as the MIS (n_S) as well as to macroscopic features such as the S factor.

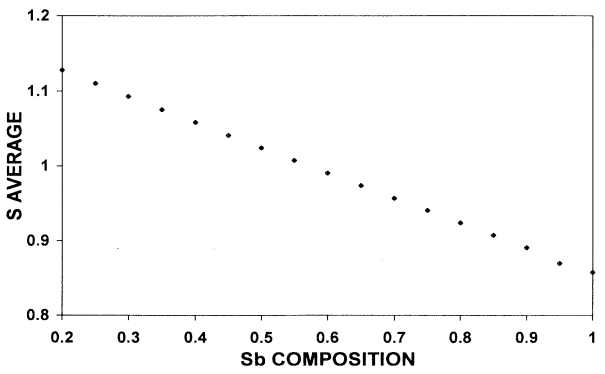

FIG. 5. Variation of the average S factor of the GaSb/GaAs heterostructure as a function of the Sb composition of the $GaAs_{1-x}Sb_x$ transitional layer.

For systems where a large lattice mismatch exists between the host materials, the strategy of growing intermediate buffer layers before arriving at the final overlayer is now being widely investigated. These transitional layers are generally alloy layers which ensure a continuous matching of the relevant features of the main host materials selected for the growth sequence. It is then important to define reliable and physically well-based criteria in order to make an optimized choice of the composition of the transitional layer. These criteria are formulated by the continuity conditions for geometric (n_S) and elastic-density factors (S). We then demonstrate that it is possible to make such optimized choices by applying the S-correlated theory of MIS's and MDNC's. One successful issue of our approach is that it enables us to predict that a transitional layer of composition $GaAs_{0.43}Sb_{0.57}$ is suitable in improving the quality of the GaSb/GaAs interface. By comparing this result with the experimental results, we show that this latter choice is a realistic choice which several years ago used the MBE growth technique.[15]

The originality of the S-correlated theory is to provide simple criteria based on simple physics relying on the elasticity theory which, applied to growth problems, enable us to make optimized choices of the constituent layers of a heterosystem. Among all these problems, we considered those related to the growth of a transitional layer (buffer layer) aimed at improving the heterostructure quality. By applying the continuity conditions imposed by the S-correlated theory of MIS's and MDNC's, we are then able to determine optimized choices in heterostructure growth.

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