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1996 J. Phys.: Condens. Matter 8 5871

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Semiconductor heterointerfaces, continuity conditions, heteroepitaxy and materials physics

P Masri† and J Siviniant

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

Received 10 April 1996

Abstract. Heteroepitaxy and host materials physics as addressed via semiconductor heterostructure fields are considered within the framework of the elasticity-based, *S*-correlated, theory of misfit-induced superstructures (MISs) and the derived continuity conditions which apply through the heterointerfaces. This enables us to optimize the choice of the host materials of the heterostructure and to gain more insight into the in-heterostructure values of the physical parameters involved in the theory. As an application, we concentrate (i) on the elastic properties (elastic constant) of the host materials of two polytype heterostructures, namely CdTe/Cd_{1-x}Zn_xTe/ZnTe and CdTe/Cd_{1-x}Mn_xTe/MnTe and (ii) on the optimization of the composition of the intermediate alloy layer. This enables us to calculate the in-heterostructure value of the elastic properties of the zinc-blende phase of MnTe.

1. Introduction

A comprehensive study of heteroepitaxy problems as addressed by modern growth techniques implies the following.

(i) A good understanding of the physics involved in the growth process. This is related to the heterointerface physics as different atomic species interact together at the early stages of the growth sequence, followed by the formation of the crystalline phases associated with the selected host materials and characterized by different lattice parameters. The consequent lattice misfit may be taken up by interface strains up to a critical layer thickness beyond which extended defects may appear as dislocations. The choice of the host materials indeed plays a dominant role in the interface problem. However, in applied physics, it is the application aimed at which mainly determines the host material choice; for example, the development of a high-temperature electronics and high-temperature devices leads us to select SiC- or GaN-based heterostructures. Having chosen the host materials, one may think of improving the heterostructure quality by applying different processings: among these, the insertion of an intermediate alloy layer or the incorporation of impurities may improve the lattice matching and also the homogeneity of the system with respect to, e.g., its elastic properties. These processings may be selected on the basis of continuity criteria involving parameters relevant to the interface problem, which interests us here. Within this framework, one can guess that the elasticity theory lies at the very heart of this problem.

† Author to whom any correspondence should be addressed: fax +67 143031; e-mail: masri@int1.univ-montp2.fr.

(ii) A good knowledge of the relevant properties of the host materials—not only the bulk properties but also the in-heterostructure properties as these bulk features may be modified by the heterostructure formation.

In what follows, we develop a strategy which enables us to investigate, at the same time and by using a self-consistent procedure, (i) growth physics, through the optimization of the heterointerface quality and system homogeneity, and (ii) the physics of the materials involved in the heterostructure.

The bulk-grown phase of MnTe exhibits the hexagonal NiAs crystal structure [1]. However, recent modern growth techniques such as molecular beam epitaxy (MBE) have shown that it is possible to stabilize the zinc-blende phase of MnTe [2]. This latter is characterized by a quite different band gap [3]: 3.18 eV (in the near ultraviolet) instead of 1.3 eV (in the near infrared) for the hexagonal phase. This new finding has renewed the interest in this material as belonging to wide-gap semiconductor family able to provide carrier confinement in semiconductor-based quantum structures for optoelectronic applications at short wavelengths.

In the case of MnTe, structural, magnetic and electronic properties of the zinc-blende phase have been investigated theoretically [3] through spin-polarized total energy calculations. However, few studies have been devoted to the determination of the elastic properties of the zinc-blende phase of MnTe when alloyed with other materials. These properties are indeed relevant to growth experiments of this material on different substrates. In [4], the elastic constants of $\text{Cd}_{1-x}\text{Mn}_x\text{Te}$ ($0 \leq x \leq 52$) and $\text{Cd}_{0.52}\text{Zn}_{0.48}\text{Te}$ have been determined at 296 K and atmospheric pressure. The lattice parameter of the alloy is, in both cases, smaller than that of CdTe. Thus, one may expect a stiffening of the elastic constants for the alloy, with respect to CdTe. This is the case for Zn-based alloy while the opposite trend is observed for Mn-based alloy.

The elastic properties are macroscopic features which are introduced by the elasticity theory of crystals: this corresponds to the wavelength limit to which the ultrasonic experimental probe belongs. This is to say that, in this case, it is a large part of the sample (of the order of magnitude of the wavelength) which is monitored and the measured behaviour corresponds to the extended part where chemically different zinc-blende phases, as well as their heterointerfaces, may coexist: these are indeed CdTe-based alloys and MnTe or ZnTe phases. The existence of the alloy-stabilized zinc-blende phase of MnTe has been demonstrated in [4]. The existence of such different phases involves necessarily interfacial problems. Consequently, one must face the important problem of the optimization of the heterointerfaces with respect to different parameters and in first place with respect to alloy composition.

Facing the need to know the elastic properties of the zinc-blende phase of MnTe, alloyed with other materials, we have considered this problem from the point of view of the formation of the heterointerfaces and of their optimization. We have discussed the opportunity of considering the interface problem for the alloy-stabilized phase of MnTe. Moreover, the interface problem is addressed by modern growth experiments in which heterostructures, constituted of materials having different lattice parameters, are made. This gives strained heterostructures for layer thickness smaller than the critical thickness h_c while extended interface defects (misfit dislocations) may appear beyond h_c . The vital problem in this field is to obtain heterostructures with high interface quality. To do so, different techniques such as the insertion of (i) strained layer superlattices [5] (SLSs), (ii) a single strained interlayer [6] (SIL), and (iii) a transitional layer introduced in order to reach a gradual matching of geometric parameters through the heterostructure, have been

tried. Examples of the third method exist for the GaSb/GaAs system where the growth of a GaAs_{1-x}Sb_x alloy epilayer on GaAs has been carried out by MBE [7–9]. In [10], we have demonstrated that this may be an efficient method for optimizing the interface quality with respect to not only geometric factors but also elastic factors which are relevant to interface defect formation.

For zinc-blende MnTe, we are also concerned by the heterointerface problem not only because of the alloy-stabilized nature of the zinc-blende phase, but also because of its incorporation in several heterostructures [2] as (i) a thick epilayer of MnTe grown on CdTe substrate or (ii) a MnTe/CdTe/MnTe single quantum well. For both systems, (i) the problem of the existence of a Cd_{1-x}Mn_xTe alloy intermediate layer due to interfacial mixing and (ii) the incorporation of such an alloy as a transitional layer to improve the interface quality are worth analysing. This implies that in such heterosystems, two heterointerfaces must be considered, namely Cd_{1-x}Mn_xTe/CdTe and Cd_{1-x}Mn_xTe/MnTe.

In what follows, we aim to optimize the choice of the composition of the alloy with respect to parameters relevant to growth experiments, which involves geometric and elastic properties of the growing phases. We will carry out the optimization self-consistently with respect to (i) the alloy composition and (ii) the elastic properties. We present the method which we use to realize such a project. Then, we apply it to zinc-blende MnTe and ZnTe-based heterostructures.

2. Method

Let us briefly recall the main points of the theory, as more details are given elsewhere [10]. Heterostructure growth raises several problems due, among other factors, to the use of lattice-mismatched host materials in building up a heterostructure. This use is imposed by the reduced number of host materials fulfilling the lattice-matching conditions. These lattice-mismatched heterostructures can be grown with essentially no misfit dislocation (MD) generation if the layer thickness is smaller than the layer critical thickness h_c . In this case, the lattice mismatch is totally accommodated by uniform lattice strains. These strains stabilize the heterointerface created by the growth experiment and, consequently, correlated chemical (the nature of the interface planes, alloying, intermixing) and geometric features (such as misfit-induced superstructure, MIS) establish at these interfaces. This correlation has been demonstrated [9] for GaAs_{1-x}Sb_x/GaAs: surface reconstructions of the alloy layer are rather GaSb-surface-like for $x \geq 0.8$ and GaAs-surface-like for $x \leq 0.5$. Therefore, a good strategy is to assess our study on the basis of a physical model which describes properly these MISs. As we will demonstrate, this physical model states that the super-unit cell (MIS) which accommodates the lattices of two interacting host layers is determined by the mismatch (i) of geometric features such as the lattice parameters [11] and (ii) of elastic constant parameters as a consequence of the application of the elasticity theory [12]. Within the framework of this theory, we may identify the S -factor, i.e. the elastic constant–density ratio $S = C_{ij}/\rho$, as an important parameter to be considered. The elasticity theory equations to which we are referring [12] are

$$\frac{\partial^2 u}{\partial t^2} = \frac{C_{11}}{\rho} \frac{\partial e_{xx}}{\partial x} + \frac{C_{12}}{\rho} \left(\frac{\partial e_{yy}}{\partial x} + \frac{\partial e_{zz}}{\partial x} \right) + \frac{C_{44}}{\rho} \left(\frac{\partial e_{xy}}{\partial y} + \frac{\partial e_{zx}}{\partial z} \right) \quad (1)$$

where u is the x -component of the displacement, ρ is the density, the C_{ij} are the elastic constants, and the $e_{\sigma\sigma'}$ are the strain components ($\sigma, \sigma' = x, y$ or z). Similar equations for y and z can be deduced from equation (1). These equations may be considered as the signature of strain-induced lattice dynamics, as the left-hand side of equation (1) is

proportional to ω^2 , the square of the angular frequency ω , and the two effects are correlated via the S -factor.

In layered structures, if we keep the lattice periodicity in the layer plane, a Fourier analysis of the dynamics in terms of Bloch waves relates ω to the components of the wave vector in the growth plane. Reconstruction effects involve band folding. Then we may find, in the wave-vector representation (Brillouin zone (BZ)) of the phonon frequencies of the heterostructure and at the limit of long wavelength where the elasticity theory applies, the signature of vibration modes originating from the short-wavelength part of the dispersion relations. At this limit, the waves may resolve the microscopic nature of the lattice. This is to say that the folded part may carry with it vibrational modes which depend upon the size of the interface BZ along the high-symmetry directions and consequently the extension of the interface superstructure. Because of the folding, the vibrational modes become part of the dispersion relations at the wavelength limit and thus the solution of the elasticity theory equations. Let us now illustrate the above analysis by writing down the mathematics which supports the physics that we have presented.

In what follows, we consider the case of a heterostructure constituted of two host materials: A (B) represents the substrate (overlayer) with a lattice parameter a_A (a_B) and an S -factor equal to S_A (S_B). The extension of the bidimensional BZ (2DBZ) associated with the surface layer lattice is scaled by the wave-vector components $g_x \sim \pi/ma$ and $g_y \sim \pi/na$ where a is the lattice parameter, x and y are in-plane symmetry directions, and m and n are integers which scale the corresponding extension of the unit cell associated with the surface lattice stabilized by a superstructure with an in-plane (x, y) periodicity. The S -correlated theory of MISs states that [10, 13]

$$\omega^2 \propto SG^{-1} \quad (2)$$

where

$$G \equiv 1/g_x g_y \propto (mn)a^2. \quad (3)$$

If we write down such a relationship for each host material A and B and if we impose phonon frequency matching between materials A and B, we end up with the fundamental equation of the S -correlated theory [13] of MISs:

$$G_B G_A^{-1} = S_B S_A^{-1} \quad (4)$$

where

$$S_{A,B} = (C_{11}/\rho)_{A,B} \quad (5)$$

and

$$G_A \propto (mn)a_A^2 \quad (6)$$

$$G_B \propto (pq)a_B^2. \quad (7)$$

G_A and G_B represent the geometric factors of the substrate and of the overlayer respectively. Let us recall that such a theory allowed us to predict interface superstructures for several heterosystems [14, 15], such as SiO_2 (Coesite)/Si, Ge/Si, a-Si/Ge_{0.2}Si_{0.8}, and Ge_{0.5}Si_{0.5}/Si. Recently, we applied this theory to study, for Si_xGe_{1-x}/Si heterostructures, the evolution of the interface superstructure as a function of the Si composition x of the alloy [13].

The lattice misfit between two materials A and B depends on the difference $\Delta = |a_A - a_B|$. The dislocations which are created when the strain relief conditions on the formation energy are fulfilled are characterized by a geometric feature, namely the associated Burgers vector [16]. At a nanometric scale, the elementary quantity which we may define is a 'small' Burgers vector $b_e = a_B - a_A$, if $a_B > a_A$: b_e represents a rather small fraction

of the lattice parameters. In the case of perfect epitaxy, this corresponds to small epitaxial dislocations. Because of a vernier effect, we end up with a network of epitaxial MDs which are fairly parallel with a lattice spacing equal to L . The density of MDs is low when Δ is small: then if $b_e \rightarrow 0$, one may expect that $L \rightarrow \infty$. Let us now assume that the periodicity in the interface plane fulfils isotropic conditions; then we have $m = n$ and $p = q$ and the MD network is a square lattice along the directions x and y . The correlation theory equation implies that the superstructure which stabilizes an interface and the associated MD network must involve geometric and elastic density (S) factors as deduced from the elasticity theory of dynamics. The dynamics is involved here because the stabilizing superstructures are obtained subsequent to interface reconstructions where atomic displacements occur, especially assisted by phonons. These reconstructions are strain correlated. Furthermore, we assume that the corresponding periodicity of the interface unit cell must match the A and B lattices via a vernier process. In this case, the atomic sites of the interface superstructure can be considered as precursor sites where ‘nucleation’ centres for MDs (MDNCs) may be formed when the formation energy of MDs becomes lower than that of misfit strain. This will result in a network of parallel MDs. The lattice spacing L of this MD network is usually obtained by applying the following geometric condition [11]:

$$(n_1 + 1)a_A = n_1a_B \quad \text{if } a_A < a_B \quad (8)$$

where n_1 is the superstructure parameter, given by the relationship

$$n_1 = a_A/(a_B - a_A). \quad (9)$$

Equation (8) holds when the B lattice is under compression and the A lattice is under extension. It states that after n_1 jumps on the B lattice and $n_1 + 1$ jumps on the A lattice, we may find in coincidence two interface sites belonging respectively to B and A. The MD spacing is then calculated by using the value of n_1 and the Burgers vector. This above method represents the geometric approach for MISs and MDNCs.

In what follows, we will extend the correlation theory [13–15] as follows. Our aim is to determine the MISs which may stabilize the A/B interface in the misfit strain regime. To do so, we introduce a superstructure parameter n_S and we express the geometric factors G_A and G_B as functions of n_S as

$$G_A \propto (n_S + 1)^2 a_A^2 \quad (10)$$

$$G_B \propto n_S^2 a_B^2 \quad \text{with } a_B > a_A. \quad (11)$$

Equations (4) to (7) and equations (10) and (11) give the relationship

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

with

$$S = S_B/S_A \quad \text{and} \quad a_B > a_A. \quad (13)$$

Equation (12) represents the S -correlated theory of MISs and of the related structural features of the MD network confined to the A/B interface.

If $S = 1$, one can see that $n_S = n_1$: the condition $S = 1$ implies that we have a matching of the elastic constant–density ratios. It is only in this case that the density of MDNCs predicted by the S -correlated theory is equal to that given by the geometric equation.

If the material A is under compression and B is under extension ($a_A > a_B$), the geometric approach gives

$$n_1 = a_B/(a_A - a_B) \quad (14)$$

while the present S -factor-correlated theory of MISs and the MD network gives

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

If the matching condition is not fulfilled for S , then $n_S < n_1$: this means that the size of the MIS and, consequently, the lattice spacings of MDNCs are smaller than those given by the geometric approach.

3. Continuity conditions at heterostructure interfaces

3.1. General considerations

When we intend to make a heterostructure for a particular application in, e.g., microelectronics or optoelectronics, we start in practice by selecting a set of materials suitable for the application aimed at. Then, we try to improve the interface quality of the chosen heterostructure by using different methods, such as the incorporation of selected impurities, annealing, or the insertion of an intermediate layer which may be an alloy of the main host materials. Different experimental techniques have been developed in order to study interfaces, to estimate their quality, to identify the nature of the defects present there and to measure the density of interface defects.

Beside these methods, it is useful to develop a theoretical strategy which may enable us to optimize the interface quality. As discussed before, this strategy may be based on the definition of some criteria which involve host material features relevant to the growth problem. In heterostructures where strains play a vital role in interface properties, we have learnt from elasticity theory that the optimization process is successful if we end up with geometric as well as elastic density properties matched at the interfaces of the heterostructure. In what follows, we will present the optimization criteria for a polytype heterostructure A/C/B.

3.2. The case of polytype heterostructures

Often, the insertion of an adequate intermediate layer C, between A and B, may improve the interface quality. For such an A/C/B system, two heterointerfaces are created, namely A/C and C/B. Each interface is characterized by a MIS parameter n_S (n_{S1} and n_{S2}) and an S -factor (S_1 and S_2). On a microscopic scale, heterointerfaces are stabilized by superstructures which accommodate the lattices of two different materials, and any stable configuration must correspond to a minimum of the energy of formation of the interface. This is to say that n_S must play the dominant role in the theory. The S -correlated theory of MISs states that n_S must depend not only on the lattice parameters but also on the S -factors. Within the framework of this theory, we may optimize the interface quality by choosing A, B and C such that the following continuity condition is fulfilled by n_S :

$$n_{S1} = n_{S2}. \quad (16)$$

In principle, the best optimization which we may obtain must meet the following continuity condition for the S -factors:

$$S_1 = S_2 = 1 \quad (17)$$

for the same conditions as for obtaining equation (16). However, and depending on the heterostructure, it may not be always possible to fulfil equations (16) and (17) at the same time and for the same conditions; in the case of polytype heterostructures, the problem is complex because we then have to match four parameters which are assumed to keep their

bulk values without any fitting procedure. Moreover, we know little about the effect of a heterointerface on, e.g., the elastic properties of the host materials. We also know little about the dependence of the alloy properties on the intrinsic properties of the alloy components, and often a linear interpolation strategy is used: we are here facing the problem of the in-heterostructure or in-alloy values of any physical parameter involved in the theory. If we aim to describe elasticity-based processes in the neighbourhood of heterointerfaces, one question that we must answer is that of how to choose an adequate strategy for estimating, if necessary, the modification of bulk parameters in considering the heterostructure. If we form a ternary alloy, such as $\text{Cd}_{1-x}\text{Mn}_x\text{Te}$, we may consider that its properties result from the coexistence of two solid phases, namely CdTe and MnTe. However, we must bear in mind that these two phases interact. This interaction may involve, e.g., electronic, electrostatic or elastic fields which may trigger a matching of their properties. For example, we may be concerned by the evolution of the elastic properties of a soft phase interacting with a stiffer phase, this evolution being induced by a mechanism of minimization of the formation energy of their interface. The study of these problems is still in its infancy.

Facing the state of art in this field, our optimization strategy will be based on an exact fulfilling of equation (16) while we must check that equation (17) is nearly verified without any fitting procedure for the bulk values of the parameters involved in the theory.

Let us now consider that our sample is probed with experimental tools which integrate a large part of the lattice: this is for example the case for the experimental conditions of the determination of elastic constants based on the use of ultrasonic waves with wavelengths of the order of $\sim 10^{-2}$ cm. The two interfaces, as present in the heterostructure A/C/B, can then be 'seen' at the same time during the same run. The measured value may then be considered as an averaged value through the part of the sample including the two interfaces. We are then entitled to replace the two interfaces by an effective medium which is characterized by an S -factor which is averaged over the two interfaces by the following simple averaging rule:

$$S_{average} = (S_1 + S_2)/2. \quad (18)$$

$S_{average}$ corresponds in fact to a reference interface. The concept of a reference medium has been used in [11] for the definition of the spacing of MDs. The continuity condition for this reference interface is

$$S_{average} = 1. \quad (19)$$

Equations (16), (17) and (19) provide the continuity conditions which enable us to optimize the choice of the heterostructure with respect to the heterointerface quality. We can take advantage of these continuity conditions in two fields relevant to heterostructures: the first one concerns the growth physics aspect while the second one concerns the in-heterostructure materials physics.

(i) The first aspect emphasizes the interface quality by optimizing the choice of the host materials of the heterostructure. Having selected a set of host materials and assumed the bulk values for all of the parameters involved, we must check to which point these conditions are fulfilled. If necessary, we can investigate the mechanisms which may improve the fit of the continuity conditions. If, e.g., C is an alloy which, when inserted in the heterostructure A/B, tends to improve the interface quality, we can seek self-consistently for the alloy composition which optimizes the system with respect to the continuity conditions. This aspect has been developed elsewhere [10].

(ii) The second aspect is related to the in-heterostructure materials physics. It is worth considering it because these continuity conditions enable us to establish a relationship

between the different interacting host materials as present in the heterostructure: this has consequences for the features of the host materials relevant to the problem considered, as these features are now correlated via (16), (17) and (19) for optimization needs. In the framework of the S -correlated theory of MISs, the relevant features are the lattice parameter a , the elastic constant C_{11} and the density ρ . We can then take advantage of the continuity conditions to calculate the in-heterostructure value of the relevant host material features.

In what follows, we will concentrate on the second aspect, although the first one is in fact inherent to the self-consistent procedure.

4. Application to heterostructures with alloyed layers

4.1. Continuity conditions and elastic constant determination

In what follows, we present the strategy on the basis of which we assess our approach, to gain some insight into the determination of the elastic constants of in-heterostructure materials. To build up a heterostructure, we use some selected host materials. An efficient use of this selection in the heterosystem often relies on a good characterization of their relevant physical properties before and after their incorporation: within the framework of the S -correlated theory of MISs, these are the lattice parameter, the density and the elastic constant. In the heterostructure, as heterointerfaces are created, this implies that the bulk values of these quantities may shift toward in-heterostructure values. As we may guess, this problem lies at the very heart of growth physics. Good growth conditions must aim to produce high-quality heterointerfaces through the matching of the host material features. This matching may be aimed at when selecting the host materials or it may be triggered during the growth process; the presence, in the heterostructure, of an alloy layer may result from the insertion of such a layer between two host materials or may be due to interfacial mixing.

In our approach, the heterointerface quality is optimized by applying continuity conditions for n_S and S throughout the whole system. In order to demonstrate the validity and the usefulness of our method, we apply it to two polytype heterostructures, namely CdTe/Cd_{1-x}Zn_xTe/ZnTe and CdTe/Cd_{1-x}Mn_xTe/MnTe. The following investigation will concentrate on the elastic constant parameter C_{11} which is involved in the S -correlated theory of MISs.

4.2. The case of CdTe/Cd_{1-x}Zn_xTe/ZnTe

The elastic constants of CdTe and ZnTe are well known: e.g., we have $C_{11}(\text{CdTe}) = 0.533 \times 10^{12} \text{ dyn cm}^{-2}$ and $C_{11}(\text{ZnTe}) = 0.713 \times 10^{12} \text{ dyn cm}^{-2}$. Their densities and their lattice parameters are respectively equal to $\rho = 5.87 \text{ g cm}^{-3}$, $a = 6.482 \text{ \AA}$ and $\rho = 5.636 \text{ g cm}^{-3}$, $a = 6.1 \text{ \AA}$. The lattice mismatch is equal to 6%. By choosing a system constituted of well characterized host materials, we aim to demonstrate the validity of our approach and to answer the following question: to what extent are the continuity conditions fulfilled when we use selected values of C_{11} , ρ and a without any fitting? Moreover, we are interested in this heterostructure because, as long as we concentrate on the elastic constant, such a behaviour has been determined in [4] for the alloy Cd_{1-x}Zn_xTe for a zinc concentration equal to $x = 0.48$.

The insertion (or the formation) of an intermediate alloy layer, such as Cd_{1-x}Zn_xTe, into CdTe/ZnTe may improve the lattice matching between these host materials. This creates two heterointerfaces, namely the alloy/ZnTe the CdTe/alloy interfaces. Thanks to

the molecular beam epitaxy (MBE) technique, it is now possible to grow $\text{Cd}_{1-x}\text{Zn}_x\text{Te}$ on different substrates with a high crystalline quality [17, 18]. It is also possible to grow by MBE ultrathin ZnTe layers in CdTe, and the morphology of the pseudomorphic layers has been characterized by high-resolution electron microscopy [19]. At the heterointerface, the ZnTe lattice is in strong extension and the CdTe lattice is in weak compression. Different configurations may be assumed for the alloy layer. (i) The first one considers a homogeneous alloy with an elastic constant C_{11} obtained by applying Vegard's law to CdTe and ZnTe. One knows that, depending on growth conditions, ZnTe islands may form on the CdTe surface. Even in this case, the system may reach such a configuration after relaxation and interdiffusion processes triggered by matching requirements. (ii) The second configuration may consist in an inhomogeneous two-phase intermediate layer of unrelaxed ZnTe and CdTe islands.

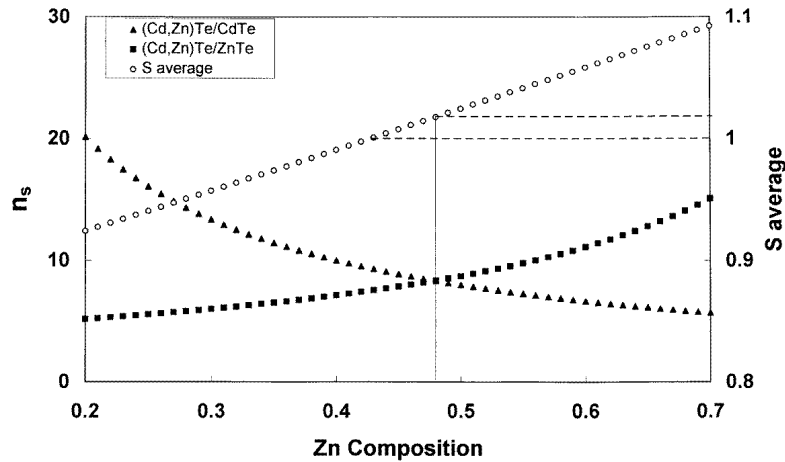


Figure 1. Variations of the MIS parameter n_S (\blacktriangle , \blacksquare) and S -average (\circ) as functions of the Zn composition of the $\text{Cd}_{1-x}\text{Zn}_x\text{Te}$ intermediate layer of the $\text{CdTe}/(\text{Cd}, \text{Zn})\text{Te}/\text{CdTe}$ heterostructure. The solid-symbol curves (\blacktriangle , \blacksquare) are respectively associated with the interfaces $(\text{Cd}, \text{Zn})\text{Te}/\text{CdTe}$ and $(\text{Cd}, \text{Zn})\text{Te}/\text{ZnTe}$. The continuity conditions correspond (i) to the crossing of curves marked with \blacktriangle and \blacksquare , and (ii) to $S_{average} = 1$.

In what follows, we consider that the first configuration prevails for the intermediate layer. We have calculated S and n_S , for each heterointerface, by choosing the values of the relevant parameters a , C_{11} and ρ as follows: (i) for each layer (CdTe, ZnTe), unchanged bulk values are assumed; and (ii) for the alloy, a linear interpolation between CdTe and ZnTe is used. The results are represented in figure 1. We discover that the continuity condition for n_S (equation (17)) is fulfilled for $x = 0.48$. This corresponds to the alloy of composition $\text{Cd}_{0.52}\text{Zn}_{0.48}\text{Te}$ considered in [4]. The corresponding MIS is equal to $n_S \cong 8$. At this composition, the S_1 - and S_2 -values are approximately equal to 1 and $S_{average} \cong 1.018$. One can see that the continuity condition for $S_{average}$ is fulfilled with a precision of $\sim 2\%$ for $x = 0.48$ when the bulk values of a , C_{11} and ρ are used. The corresponding alloy value of C_{11} is equal to $0.62 \times 10^{12} \text{ dyn cm}^{-2}$, in agreement with the value ($0.6 \times 10^{12} \text{ dyn cm}^{-2}$) reported in [4] for 296 K and at atmospheric pressure. We then conclude that the bulk values of a , C_{11} and ρ for CdTe and ZnTe fulfil the continuity condition for n_S when an alloy layer of Zn composition $x = 0.48$ is inserted: this composition is the one which has been aimed at in [4]. In previous work [10] on the heterostructure $\text{GaSb}/\text{GaSb}_x\text{As}_{1-x}/\text{GaAs}$, we

have also found that the continuity conditions were fulfilled for an Sb composition equal to $x = 0.57$ and we discovered that the corresponding alloy composition has been aimed at in a MBE experiment [8].

We also found that the continuity condition for $S_{average}$ is exactly fulfilled for $x = 0.43$. We may then conclude that an intermediate composition x between 0.43 and 0.48 will provide a heterostructure with heterointerfaces matching the continuity conditions with a high degree of precision.

In the above application, we have used the bulk values of the host material parameters. The ensuing conclusion is that, in particular, the bulk values of C_{11} for CdTe and ZnTe, when used in the heterostructure, enable us to verify the continuity conditions for n_S and $S_{average}$. We also found that these two conditions are nearly, but not exactly, fulfilled for the same Zn composition.

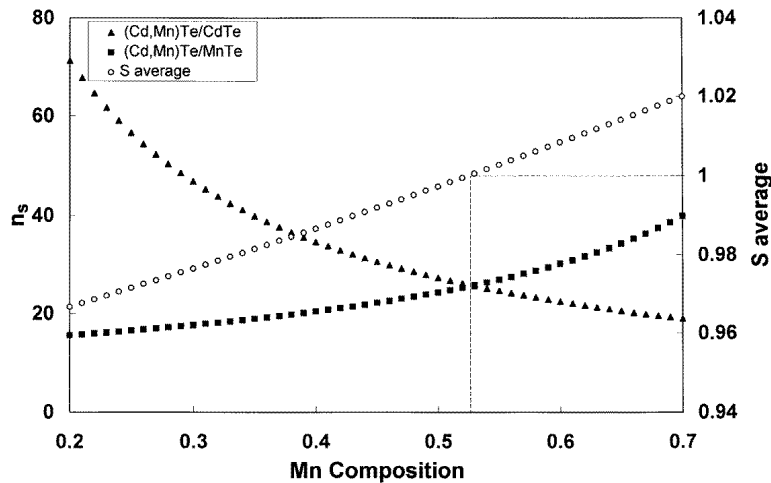


Figure 2. The same as figure 1, but for the CdTe/(Cd, Mn)Te/MnTe heterostructure.

4.3. The case of CdTe/Cd_{1-x}Mn_xTe/MnTe

MBE has been used to grow zinc-blende MnTe films on CdTe [20]. The insertion of an intermediate alloy layer of Cd_{1-x}Mn_xTe may be used with the aim of improving the CdTe/MnTe interface quality, besides inducing new properties by incorporating the magnetic ions Mn in CdTe. Moreover, even in the binary heterostructure CdTe/MnTe, one may expect to have an alloyed transitional layer due to interface mixing. In such a system, two heterointerfaces are involved. In [4], the elastic constants of Cd_{1-x}Mn_xTe have been determined and the values are given for three Mn compositions, $x = 0.06, 0.45$ and 0.52 . For the highest values of x , C_{11} is equal to 0.51×10^{12} dyn cm⁻². If one assumes Vegard's law, the alloy values of, e.g., C_{11} , given in [4], may be obtained by using for MnTe a value of C_{11} equal to 0.49×10^{12} dyn cm⁻².

In applying the S -correlated theory of MISs and the consequent continuity conditions to this heterostructure, we aim to answer the following question: can we optimize the CdTe/MnTe interface with the transitional alloy layer considered and, if this is possible, what are the corresponding correlated values of the Mn composition and of the elastic constant C_{11} of the alloy? This problem is the inverse of the one considered in subsection

4.2. Here, we start off by assuming that the continuity conditions are fulfilled and we intend, among other things, to determine the in-heterostructure value of the elastic constant C_{11} of the alloy and, eventually, the in-heterostructure value of C_{11} of the zinc-blende phase of MnTe.

We have carried out a self-consistent procedure which involves the continuity conditions for n_S , S , and the elastic constant C_{11} of MnTe. The results are represented in figure 2. We can see that the continuity condition for n_S is fulfilled for a Mn composition $x \cong 0.53$, where the crossing of n_{S1} and n_{S2} occurs for $n_S \cong 26$. Moreover, for this concentration, the continuity condition for $S_{average}$ is fulfilled. The value of the elastic constant C_{11} of MnTe which enables us to achieve the self-consistent procedure is $C_{11} \cong 0.482 \times 10^{12}$ dyn cm⁻². If we assume that the elastic constant C_{11} of Cd_{1-x}Mn_xTe may be calculated by using a linear interpolation between CdTe and MnTe, we find, for $x = 0.534$, $C_{11} \cong 0.506 \times 10^{12}$ dyn cm⁻². On the whole, our results are in good agreement with those given in [4]. Let us recall that our strategy for determining C_{11} is based on the application of the continuity conditions for the heterointerfaces of the system under study. From this point of view, we say that the calculated value of C_{11} is the in-heterostructure value of C_{11} of the zinc-blende phase of MnTe.

5. Conclusion

The S -correlated theory of MISs [13–15] enables us to predict which superstructure may stabilize the heterointerfaces of heterostructures where interface strains play a dominant role. The extension of this theory to growth problems has led to the formulation of interface continuity conditions involving the superstructure parameter n_S and the elastic constant-density factor S as present in the elasticity theory of lattice dynamics. The application of these conditions to the heterostructure field results in two issues.

(i) The first issue is relevant to growth physics: by selecting the host components of a heterostructure in order to fulfil the continuity conditions, we may optimize the heterostructure choice with respect to the interface quality.

(ii) The second issue is relevant to the physics of the materials involved in the heterostructure: this is in practice done by carrying out a self-consistent procedure which implies the fulfilling of the continuity conditions and an iteration process involving the host material property to be determined.

We have applied our approach to two heterostructures, namely CdTe/Cd_{1-x}Zn_xTe/ZnTe and CdTe/Cd_{1-x}Mn_xTe/MnTe. The first one is considered in order to establish the ability of the S -correlated theory of MISs and its consequent continuity conditions to properly study growth and host materials physics problems. The second system is considered in order to gain more insight into the elastic properties of the zinc-blende phase of MnTe. We demonstrate that it is possible, by fulfilling the continuity conditions, to determine the elastic properties of the host materials of the heterostructure. The results that we obtain are in good agreement with the experimental results [4]. Moreover, our approach may afford the possibility of reaching a better understanding of the in-heterostructure values of the parameters relevant to the S -correlated theory of MISs. These latter may be not very different from the bulk values: this is, e.g., the case for ZnTe-based heterostructure as we find that, if we keep the bulk values of the elastic constant C_{11} of CdTe unchanged, we may optimize the composition of the alloy Cd_{1-x}Zn_xTe with the bulk value of C_{11} of ZnTe. Here, we deal with a host material (ZnTe) which is stiffer than the embedding material (CdTe). The situation seems to be different for the MnTe-based heterostructure, as we may

expect that MnTe will be softer than CdTe. The point is that the in-heterostructure shifts of the elastic properties of the host materials do indeed depend on their relative bulk values.

References

- [1] Allen J W, Lucovsky G and Michelsen J C Jr 1977 *Solid State Commun.* **24** 367
- [2] Durbin S M, Han J, Sungki O, Kobayashi M, Menke D R, Gunshor R L, Fu Q, Pelekanos N, Nurmikko A V, Li D, Gonsalves J and Otsuka N 1989 *Appl. Phys. Lett.* **55** 2087
- [3] Wei S H and Zunger A 1986 *Phys. Rev. Lett.* **56** 2391
- [4] Maheswaranathan P, Sladek R J and Debska U 1985 *Phys. Rev. B* **31** 5212
- [5] See, for example,
Soga T, Jimbo T and Umeno M 1990 *Appl. Phys. Lett.* **56** 1433
- [6] Okuno Y and Kawano T 1994 *J. Cryst. Growth* **145** 338
- [7] Zhao J H, Li A Z, Jeong J, Wong D, Lee J C, Milliman M L, Schlesinger Y E and Milnes A G 1988 *J. Vac. Sci. Technol. B* **6** 627
- [8] Waho T, Ogawa S and Maruyama S 1977 *Japan. J. Appl. Phys.* **16** 1875
- [9] Chang C A, Ludeke R, Chang L L and Esaki L 1977 *Appl. Phys. Lett.* **31** 759
- [10] Masri P 1995 *Phys. Rev. B* **52** 16627
- [11] See, for example,
Matthews J W 1975 *Epitaxial Growth, Part B* (New York: Academic) p 505
- [12] See, for example,
Kittel C 1968 *Introduction to Solid State Physics* 3rd edn (New York: Wiley) p 119, equation (31)
- [13] Masri P 1994 *Phys. Rev. B* **49** 2185
- [14] Masri P 1988 *Phys. Rev. B* **37** 8462
- [15] Masri P 1989 *Phys. Rev. B* **39** 10384
- [16] Friedel J 1967 *Dislocations* (Reading, MA: Addison-Wesley)
- [17] Olego D J, Faurie J P, Sivanathan S and Raccach P M 1985 *Appl. Phys. Lett.* **47** 1172
- [18] Dinan J H and Qadri S B 1985 *J. Vac. Sci. Technol. A* **3** 851
- [19] Jouneau P M, Tardot A, Feuillet G, Mariette H and Cibert J 1994 *J. Appl. Phys.* **75** 7310
- [20] Bressler P R and Gumlich H-E 1994 *J. Cryst. Growth* **138** 1028