PHYSICAL REVIEW B VOLUME 39, NUMBER 14 15 MAY 1989-I

Theoretical contribution to the study of an a-Si/Ge$_{0.2}$Si$_{0.8}$(111) interfacial structure

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(Received 23 June 1988; revised manuscript received 17 January 1989)

A recently discovered correlation between geometric and elastic-density factors to determine the interfacial superstructure of an a-Si/Ge$_{0.2}$Si$_{0.8}$(111) heterostructure subsequent to film growth is applied and the results are compared with experimental data obtained by synchrotron x-ray diffraction.

I. INTRODUCTION

Modern growth techniques, such as molecular-beam epitaxy, have led to the fabrication of heterostructures presenting very well-controlled features relevant for semiconductor devices. The current experimental studies of their physical properties are increasingly showing the importance for such systems of solid-solid interfaces of the heterostructure junctions. One aspect of this problem is, for example, the control of interface composition which is relevant to heterostructure band-gap engineering. The case of a graded Al$_x$Ga$_{1-x}$As/GaAs heterojunction has been considered and Auger depth profiling of Al and Ga concentrations within the interface region has been recorded.[1] In order to understand the results of such a process, many solid-state feature modifications characteristic of composition-graded interfaces have to be taken into account, such as (i) the modification of lattice parameters,[2] and consequently the variable lattice matching between the materials forming the heterojunction; this is associated with built-in strain in the pseudomorphic growth regime, and (ii) the modification of the heterostructure band gap,[3] important because of its relevance to heterojunction band-gap engineering.

The knowledge of the interface lattice microscopic structure is also important. This structure is related to the symmetry of the interfacial unit cell and may involve reconstruction processes experienced by the initial substrate-surface structure subsequent to overlayer growth. These processes might be relevant to interfacial electronic properties, electric properties, and the ensuing consequences for device applications. As far as surface structure is concerned, the development of experimental techniques such as low-energy electron diffraction (LEED),[4,5] reflection high-energy electron diffraction (RHEED),[6] and scanning tunneling microscopy (STM),[7] allows a detailed knowledge of surface structural properties and their evolution under such experimental processing techniques as annealing and adsorption. However, LEED, for example, can probe only the top surface layer and can therefore provide no information about the inner solid-solid interface as it exists in heterostructures. For such investigations, techniques that penetrate beyond the first film layers are required. Synchrotron grazing-incidence x-ray diffraction has been used to obtain structural information about solid-solid interfaces, for example, in the case of a-Si/Ge$_{0.2}$Si$_{0.8}$(111),[8] where it was shown that the initial GeSi(111) 5×5 substrate superstructure is preserved after deposition of an amorphous-silicon overlayer. As these interfacial structure studies appear, it is useful to try to understand the mechanism of interfacial superstructure modifications subsequent to film-epitaxial-growth conditions.

Recently, we reported the discovery of a new simple correlation between geometric and elastic-density factors associated with interfacial structure modifications subsequent to epitaxial-growth conditions of films on crystalline-substrate surfaces.[9] One class of heterostructures for which this correlation operates concerns heterojunctions, the interface of which develops strain fields due to the lattice-parameter mismatch between the two materials forming the heterojunction. This strained-interface region may involve growing films of thicknesses smaller than the critical thickness, beyond which extended defects are created. The geometric factor G of the correlation is defined as the ratio of the substrate-surface unit-cell size to the interface unit-cell size after creation of the heterostructure. The elastic-density factor S is the ratio of elastic constant to density parameters associated with substrate and overlayer materials. In its simple formulation, the correlation implies a similarity between G and S, i.e., $R \equiv S/G = 1$.

In this study, we will demonstrate that the use of this correlation enables us to predict the interfacial superstructure of an a-Si/Ge$_{0.2}$Si$_{0.8}$ heterostructure and we will compare our result with recent experimental data in a synchrotron x-ray-diffraction study.[8]

II. A SIMPLE STATEMENT OF THE CORRELATION

We will refer to Ref. 9 for all definitions and notations. Two main features are relevant to such strain-stabilized interfacial superstructures. The elastic-density factor $S = C_{ij}/\rho$, as it is present in the elasticity theory, relates the strain to crystal dynamics. For example, for cubic crystals we have[10]

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

where u is the x component of the displacement, ρ is the density, C_{ij} are the elastic constants, and $e_{\sigma\sigma}$ the strain components. The equations for the directions y and z are deduced by symmetry. Equation (1) is a useful tool in recognizing the factor (C_{ij}/ρ) which links the strain components, via their derivatives, to lattice-dynamical features such as $\partial^2 u/\partial t^2$, which is proportional to the square of the frequency.

The interface unit-cell symmetry (superstructure) is involved through the wave-vector (g) representation (reciprocal lattice) within the framework of the associated first Brillouin zone. At the zone boundary, we have the relationship $g \sim \pi/na$, where n is the number which scales the length (na) of the $n \times n$ superstructure unit cell.

The phonon frequency clearly depends on the quantities S and g as $\omega^2 \sim C_{ij}/\rho G$ with $G = 1/g^2 \sim (n \times n)a^2$. We recognize that ω^2 is the ratio of the elastic-density factor to the geometric factor as in the correlation equation. Moreover, it is now well established that phonons may be used to study interfacial-structure stability and to predict stable superstructures.[11] The occurrence of these superstructures produces a folding of the phonon-dispersion relations and it has been demonstrated[11] that the vibrational spectrum associated with a final superstructure may be inferred by folding the spectrum associated with the structure from which it originates. It then appears that the correlation equation may be derived from a phonon-frequency matching relationship between materials A and B as

$$C_{11\,A}/\rho_A G_A = C_{11\,B}/\rho_B G_B \tag{2}$$

and consequently $R \equiv S/G = 1$.

The argument discussed here is complementary to that given previously[9] where the correlation was successfully applied to several interfacial superstructures. In what follows, we will demonstrate that the correlation can be used to predict interfacial structure.

III. APPLICATIONS: INTERFACIAL STRUCTURE OF a-Si/Ge$_{0.2}$Si$_{0.8}$(111)

The similarity between the geometric (G) and the elastic-density (S) factors implies that

$$G_A = \frac{S_A}{S_B} G_B \; . \tag{3}$$

This expression relates the final interfacial structure feature (G_A), accommodated by materials A and B, to the substrate structure (G_B), through the elastic-density factor S. The latter can be calculated from material bulk properties. By knowing the initial substrate surface structure G_B, Eq. (3) enables us to calculate G_A and consequently p and q, which determine the interfacial superstructure $p \times q$.[9]

Let us apply this program to the interface a-Si/Ge$_{0.2}$Si$_{0.8}$(111) which has been studied by using synchrotron x-ray-diffraction technique.[8] First of all, we must calculate the elastic-density factor,

$$S \equiv S_A/S_B = \frac{C_{11\,A}}{\rho_A} \Big/ \frac{C_{11\,B}}{\rho_B} \; , \tag{4}$$

i.e., the parameters $C_{11\,A,B}$ and $\rho_{A,B}$.

A. Alloy parameters

The alloy density ρ_B, as well as the lattice constant a_B, have been measured throughout the entire alloy system.[12] For a 20% Ge alloy, the experimental data give $\rho_B \cong 3.0075$ g cm^{-3} and $a_B \cong 5.472$ Å. We may also calculate these parameters using a rule of averaging, i.e.,

$$\rho_B = 0.2\rho_{\mathrm{Ge}} + 0.8\rho_{\mathrm{Si}} \; , \tag{5a}$$

$$a_B = 0.2a_{\mathrm{Ge}} + 0.8a_{\mathrm{Si}} \; , \tag{5b}$$

with $\rho_{\mathrm{Ge}} \cong 5.36$ g cm^{-3}, $\rho_{\mathrm{Si}} \cong 2.33$ g cm^{-3}, $a_{\mathrm{Ge}} \cong 5.658$ Å, and $a_{\mathrm{Si}} \cong 5.431$ Å. This gives

$$\rho_B \cong 2.94 \text{ g cm}^{-3}, \quad a_B \cong 5.476 \text{ Å} \; .$$

These values are in reasonable agreement with experimental data. This shows that such an averaging rule is meaningful. Although the validity of this averaging rule for elastic-constant determination has not been demonstrated, it seems reasonable to use it as a first-order approximation.[13] Therefore, we can use it to calculate the alloy elastic constant. We then obtain $C_{11\,B} \cong 1.59 \times 10^{12}$ dyn cm^{-2}. We now have all elements required to calculate the alloy elastic-density factor. We find

$$S_B \cong 0.54 \times 10^{12} \text{ cm}^2\,\text{sec}^{-2} \; . \tag{6}$$

B. a-Si parameters

Experimental data on amorphous Si (Refs. 14 and 15) have shown that the density $\rho_{a\text{-Si}}$ and Young's modulus $E_{a\text{-Si}}$ are related to the crystalline-state values $(\rho_{c\text{-Si}}, E_{c\text{-Si}})$ by the following relationships:

$$\rho_{a\text{-Si}} = 0.95\rho_{c\text{-Si}} \; , \tag{7a}$$

$$E_{a\text{-Si}} = 0.73E_{c\text{-Si}} \; , \tag{7b}$$

where

$$E_{c\text{-Si}} \cong 1.7 \times 10^{12} \text{ dyn cm}^{-2} \; .$$

We then obtain

$$\rho_A \equiv \rho_{a\text{-Si}} \cong 2.21 \text{ g cm}^{-3}$$

and consequently

$$a_A \equiv a_{a\text{-Si}} \cong 5.525 \text{ Å} \; ,$$

while the elastic constant $C_{11\,a\text{-Si}}$ (Ref. 16) may be estimated from the crystalline-state value by using the same deficit factor as that given in Eq. (7b). This gives

$$C_{11\,\mathrm{A}} \equiv C_{11\,a\text{-Si}} \cong 1.21 \times 10^{12} \text{ dyn cm}^{-2} \; .$$

It is now possible to calculate the film elastic-density factor S_A. We find

$$S_A \cong 0.55 \times 10^{12} \text{ cm}^2\,\text{sec}^{-2} \; . \tag{8}$$

It is worth noticing that this value is very close to S_B. As we will see, this has important consequences for interfacial structure.

C. *a*-Si/$Ge_{0.2}Si_{0.8}$ interface structure

The RHEED pattern from the $Ge_{0.2}Si_{0.8}(111)$ substrate surface has revealed a 5×5 superstructure.[8] This enables us to calculate the substrate geometric factor G_B. Eventually, Eqs. (3), (6), and (8) give

$$p\times q=25\ .$$

This demonstrates that the 5×5 superstructure is a possible candidate for an *a*-Si/$Ge_{0.2}Si_{0.8}(111)$ interfacial structure. This is in agreement with the recent experimental determination of an *a*-Si/$Ge_{0.2}Si_{0.8}(111)$ interfacial superstructure using the synchrotron x-ray-diffraction technique.[8]

This result indicates that the initial 5×5 substrate superstructure, as revealed by the RHEED pattern, is preserved after deposition of a 100-Å-thick *a*-Si film at room temperature. It implies the similarity between geometric and elastic-density factors, i.e., $R=1$. The system studied in this work provides a successful new test of this correlation,[9] in the sense that, now, the initial substrate structure survives in film-growth conditions.

IV. CONCLUSION

While the investigations on surface structures have now matured, due in part to the development of surface techniques (e.g., LEED, RHEED, STM, etc.), the studies of interfacial structures are still in their infancy, requiring specific nondestructive probes which penetrate these structures more deeply to reach their interface. This is an interesting topic because of the important role played by the interface on device characteristics. Local (interfacial) solid-state features are strongly involved, although bulk properties may be relevant too. Recently, we discovered[9] a correlation between geometric and elastic-density factors for heterostructures for which interfacial structures are stabilized by interfacial strains which take up the lattice mismatch between the materials forming the heterojunction. In this study, we show, by applying the correlation, that the interfacial structure of *a*-Si/$Ge_{0.2}Si_{0.8}(111)$ is the 5×5 superstructure in accordance with the experimental result.[8] We hope that this new idea will be useful in the understanding of film growth. For the class of strained-interface systems considered, the correlation, in its simplest formulation, is satisfied. There is no doubt that further experimental studies, carried out on new systems, will be very useful in the understanding of interfacial-structure formation, and consequently, in the understanding of film-growth mechanisms.

ACKNOWLEDGMENTS

Laboratoire d'Etudes des Surfaces, Interfaces et Composants associé au Centre National de la Recherche Scientifique (UA No. 040787).

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[13] This may be illustrated by the following example: in the case of AlAs, the average rule gives $C_{11}=0.5C_{11\,\mathrm{Al}}+0.5C_{11\,\mathrm{As}}\cong1.2\times10^{12}$ dyn cm^{-2}, while the elastic constant of the compound (AlAs) is $C_{11}\cong1.25\times10^{12}$ dyn cm^{-2}.

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[15] An experimental study has shown that the highest density achieved in a real amorphous-Si film may be equal to (0.97±0.2) times the crystalline density [see M. H. Brodsky, D. Kaplan, and J. F. Ziegler, Appl. Phys. Lett. **21**, 305 (1972)].

[16] A separate evaluation of $C_{11\,a\text{-Si}}/C_{11\,c\text{-Si}}$ based on the relationship between C_{11} and the two force constants α and β of Keating's model [see R. Alben, D. Weaire, J. E. Smith, Jr., and M. H. Brodsky, Phys. Rev. B **11**, 2271 (1975)] gives $C_{11\,a\text{-Si}}/C_{11\,c\text{-Si}}\cong0.8$, a value in accordance with the deficit factor (0.73) used to calculate $C_{11\,a\text{-Si}}$ from the crystalline value of C_{11}.