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Variational method applied to determine the lattice parameter profiles in semiconductor heterostructures

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We have obtained the lattice parameter profiles for Ge/Si $(1\,1\,n)$ and InAs/GaAs $(1\,1\,n)$ heterostructures using the elasticity continuum theory in the linear approximation. In our model we assume that a small fraction of the substrate participates in the heterostructures relaxation in the non-rigid approximation. Minimization of the free energy by the Euler–Lagrange method allows us to predict the evolution of the lattice parameter with the film coverage. A sigmoidal-like law for the lattice parameter profile is observed in the rigid and non-rigid approximations. This behaviour is qualitatively similar to that obtained for lower Miller indices in Ge/Si and InAs/GaAs heterostructures. As the aspect ratio changes, we observed a significant dependence of the lattice parameter slope basically for higher aspect ratio values. Therefore, the difference in the depletion parameter does not sensitively affect the lattice parameter changes for higher aspect ratios in some range of investigated materials. So the aspect ratio is seen to play a key role in relaxation mechanisms and can explain different shapes observed in the formation of heterostructures. From these results, we have deduced that the aspect ratio and subsequently the misfit strain and substrate orientations are the key parameters in relaxation processes, since they define changes in the lattice parameter with the height of deposited film.

1. Introduction

As it is well established, one of the factors which greatly influences the Stranski–Krastanov (S–K) growth mode in low-dimensional strained heterostructures is the substrate orientation. A change in the Miller indices of the substrate allows us to control the strain relaxation in the heteroepitaxial systems, consequently inducing modifications in the onset of the S–K growth mode, or even, in some cases, the inhibition of this mode. For instance, RHEED and STM measurements of InAs grown on GaAs $(0\,1\,1)$ and GaAs $(1\,1\,1)$ surfaces revealed that the growth is always two-dimensional; i.e., layer by layer, and strain is relieved by the formation of misfit dislocations [1]. However, when InAs epitaxial layers were grown on high-index substrates such as $(1\,1\,3)$ and $(1\,1\,5)$ GaAs, the PL spectra indicated a delay in the three-dimensional mode onset [2]. On the other hand, appropriate changes of substrate orientation induce different morphologies of the islands for the same epitaxial film. This phenomenon is observed by STM in Ge/Si $(0\,0\,1)$ and Ge/Si $(1\,1\,1)$ quantum dots (QDs) [3]. In our previous works [4,5], we reported theoretical studies to analyze the substrate orientation effects on S–K growth mode and electronic properties of Ge/Si $(1\,1\,1)$ and InAs/GaAs $(1\,1\,n)$ with $n = 1, 3, 5$. In these works, a semiempirical height-dependent lattice parameter was introduced as a good approximation of the lattice relaxation, in agreement with some observed experimental lattice misfit dependence with the height of the deposited film [6,7]. This model has allowed Sfaxi et al. [8] to explain the dependence of the formation process and strains on the growth temperature of the InAs QDs on $(1\,1\,3)$A GaAs substrate.

Attending to the S–K growth mode, it is known that mechanisms based on wetting interactions between the film and the substrate can terminate coarsening of the surface structures. Boundary-layer and glued wetting-layer models for the last mechanism have been reported in the literature, where variation of the surface energy, misfit or lattice parameter with film height is considered [9–11]. Focusing on the lattice parameter, in order to explain the anomalous X-ray diffraction on InAs/GaAs QDs, Schülli et al. [6,7] performed a fit of the diffraction curves where they assumed that the lattice parameter is allowed to relax monotonically from a_{GaAs} towards a_{InAs}. The resulting lattice parameter profile shows a sigmoidal-like behaviour as a function of the height above the substrate. On the other hand, Budiman and Ruda [12], in their analysis of the transition thickness, suggest that the lattice parameter of the film relaxes towards its bulk-like value. Dvurechenskii et al. [13] measured the variation of the Ge lattice

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constant during conventional MBE of Ge on Si (0 0 1) and MBE with 100 eV Ge$^+$ pulsed ion beam actions. In both measurements, they clearly observed a sigmoidal-like behaviour beginning from the 2D-to-3D transition thickness and starting to saturate at around 10 monolayers of deposited Ge layers. Etgens et al. [14] also obtained experimentally a sigmoidal law for the lattice parameter profile in MnAs/GaAs (1 1 1) heterostructures. In our previous work, we reported theoretical analysis of the parameter profile using elasticity continuum theory in Ge/Si (0 0 1) and InAs/GaAs (0 0 1) QDs for different values of the aspect ratio, where a sigmoidal-like law is obtained for the parameter profiles [15]. Once we have demonstrated that the lattice profile can be deduced from a somewhat rigorous Euler–Lagrange calculations in Ge/Si (0 0 1) and InAs/GaAs (0 0 1) QDs, the aim of the present work is to complete the latter calculations by extending our model to Ge/Si (1 1 n) and InAs/GaAs (1 1 n) heterostructures for $n = 1$, 3, 5. For this occasion, the main issue is to discuss how the change in substrate orientation can affect or not the sigmoidal-like profile obtained in the previous work [15] and to find out the relationship between the rigid or the non-rigid approximations and the shape of the lattice profile. Minimization of the free energy by the Euler–Lagrange method leads to a couple ofsecond-order differential equations with constants coefficients for the variation of the lattice parameter in the non-rigid approximation; the rigid substrate approximation provides a unique differential equation. In both rigid and non-rigid approximations, a sigmoidal-like profile is obtained for the lattice parameters in an analogous manner as that obtained for lower Miller indices. Through all the calculations, we assume a coherent behaviour of the heterostructures at the film–substrate interface without taking into account the kinetic aspects of growth mechanisms.

With this purpose, this paper is organized as follows. In Section 2, a brief description of the theoretical model is given, with special attention to Euler–Lagrange method applied for the different substrate orientations. To emphasize this, we separate our model into two basic approximations: the non-rigid and the rigid substrate approximations. The former was introduced to account for the changes in the substrate materials created by the film coverage, while the latter supposes that all the misfit strain is located in the film during the growth process. The implementation of the model in Ge/Si (1 1 n) and InAs/GaAs (1 1 n) heterostructures and the comparison with Ge/Si (0 0 1) and InAs/GaAs (0 0 1) heterostructures are discussed in Section 3. The main remarks and conclusion of this work will be given in Section 4.

2. Theoretical model

The driving force for the self-organization processes during heteroepitaxial growth is the misfit between the crystal lattice of the growing layer and that of the substrate, which creates strain in the growing layer. During growth, elastic relaxation of the internal elastic energy may take place leading to self-organized nanostructures. Knowledge of the strain field is important for understanding the creation of an equilibrium dot shape, among other things. In general, two basic approaches are used both for the calculation of the strain distribution and for the shape and island profile simulations. These approaches consist of continuum elasticity and atomistic simulations. In the elasticity continuum theory, the structure under investigation is considered as an elastic continuum and the physical parameters under study are obtained by solving the elasticity equilibrium equations or by minimizing the elastic energy stored in the system. For our analysis, we will focus on the minimization of the density volume elastic energy. Let us denote by $h(x, y)$ the deposited film thickness, i.e., the height profile, where (x, y) represent the coordinates of the planar film–substrate interface. To deduce the lattice parameter profile, we assume that all the changes are derived from the elastic density energy and we analyze both the non-rigid and the rigid substrate approximations. Within the elasticity continuum theory in linear approximation [15,16], the elastic free energy density for a thin volume layer is expressed by [17]

$$f_e = \tfrac{1}{2} C_{ijkl} u_{ij} u_{kl} \tag{1}$$

where C_{ijkl} is the stiffness tensor and u_{ij} is the strain tensor defined in terms of the derivatives of the displacement vector $\mathbf{u}$, i.e., $u_{ij} = u_{ji} = \frac{1}{2}(\partial_i u_j + \partial_j u_i)$. Indeed, as reported in our previous works, the film and substrate displacement vector components are defined in terms of height-dependent lattice parameters $a_f(z)$ and $a_s(z)$, with a_f and a_s denoting their respective bulk values [5,15].

2.1. Non-rigid substrate approximation

In the non-rigid we assume that both the deposited film and the substrate are deformed by misfit strain, so that the elastic energy is stored in the film and in the substrate. In their displacement vector components will figure out both the $a_f(z)$ and the $a_s(z)$.

For any arbitrary crystal orientation, the four-rank tensor C_{mnop} can be obtained from the (0 0 1) stiffness tensor C_{ijkl} following the relation

$$C_{mnop} = a_{mi} a_{nj} a_{ok} a_{pl} C_{ijkl} \tag{2}$$

where $a_{\alpha,\beta}$ ($\forall \alpha, \beta \in \{1, 2, 3\}$) are the rotation matrix elements and they are given in Ref. [5]. For cubic crystals such as InAs, GaAs, Ge or Si, the unique non-zero stiffness constants are c_{11}, c_{12} and c_{44}. The elastic free-energy density for any cubic system and for orientations (1 1 1), (1 1 3) and (1 1 5) are, respectively, given by

$$\begin{aligned} f_{(1\,1\,1)} = {} & c_{11}(\tfrac{1}{4}(u_{11}^2 + u_{22}^2) + \tfrac{1}{6}u_{33}^2 + \tfrac{1}{6}u_{11}u_{22} + \tfrac{1}{3}(u_{11} + u_{22})u_{33} \\ & + \tfrac{1}{3}u_{12}^2 + \tfrac{2}{3}(u_{23}^2 + u_{31}^2)) \\ & + c_{12}(\tfrac{1}{4}(u_{11}^2 + u_{22}^2) + \tfrac{1}{3}u_{33}^2 + \tfrac{5}{6}u_{11}u_{22} + \tfrac{2}{3}(u_{11} + u_{22})u_{33} \\ & - \tfrac{1}{3}u_{12}^2 - \tfrac{2}{3}(u_{23}^2 + u_{31}^2)) \\ & + c_{44}(\tfrac{1}{2}(u_{11}^2 + u_{22}^2) + \tfrac{2}{3}u_{33}^2 - \tfrac{1}{3}u_{11}u_{22} - \tfrac{2}{3}(u_{11} + u_{22})u_{33} \\ & + \tfrac{2}{3}u_{12}^2 + \tfrac{2}{3}(u_{23}^2 + u_{31}^2)) \end{aligned}$$

$$\begin{aligned} f_{(1\,1\,3)} = {} & c_{11}(\tfrac{153}{484}(u_{11}^2 + u_{22}^2) + \tfrac{3}{242}u_{33}^2 + \tfrac{51}{242}u_{11}u_{22} \\ & + \tfrac{1}{11}(u_{11} + u_{22})u_{33} + \tfrac{51}{121}u_{12}^2 \\ & + \tfrac{2}{11}(u_{23}^2 + u_{31}^2)) + c_{12}(\tfrac{89}{484}(u_{11}^2 + u_{22}^2) + \tfrac{3}{121}u_{33}^2 \\ & + \tfrac{191}{242}u_{11}u_{22} + \tfrac{2}{11}(u_{11} + u_{22})u_{33} \\ & - \tfrac{51}{121}u_{12}^2 - \tfrac{14}{121}(u_{23}^2 + u_{31}^2)) + c_{44}(\tfrac{89}{242}(u_{11}^2 + u_{22}^2) \\ & + \tfrac{6}{121}u_{33}^2 - \tfrac{51}{121}u_{11}u_{22} \\ & - \tfrac{14}{121}(u_{11} + u_{22})u_{33} + \tfrac{140}{121}u_{12}^2 + \tfrac{30}{121}(u_{23}^2 + u_{31}^2)) \end{aligned}$$

and

$$\begin{aligned} f_{(1\,1\,5)} = {} & c_{11}(\tfrac{113}{324}(u_{11}^2 + u_{22}^2) + \tfrac{209}{486}u_{33}^2 + \tfrac{113}{486}u_{11}u_{22} \\ & + \tfrac{17}{243}(u_{11} + u_{22})u_{33} + \tfrac{113}{243}u_{12}^2 \\ & + \tfrac{34}{243}(u_{23}^2 + u_{31}^2)) + c_{12}(\tfrac{49}{324}(u_{11}^2 + u_{22}^2) + \tfrac{17}{243}u_{33}^2 \\ & + \tfrac{373}{486}u_{11}u_{22} + \tfrac{226}{243}(u_{11} + u_{22})u_{33} \\ & - \tfrac{113}{243}u_{12}^2 - \tfrac{34}{243}(u_{23}^2 + u_{31}^2)) + c_{44}(\tfrac{49}{162}(u_{11}^2 + u_{22}^2) \\ & + \tfrac{34}{243}u_{33}^2 - \tfrac{113}{243}u_{11}u_{22} \\ & - \tfrac{34}{243}(u_{11} + u_{22})u_{33} + \tfrac{260}{243}u_{12}^2 + \tfrac{418}{243}(u_{23}^2 + u_{31}^2)) \end{aligned}$$

so that the total free energy for any orientation (1 1 n) ($n = 1$, 3, 5) can be expressed as

$$F_{11n} = \int\!\!\int\!\!\int_V [f_{f(1\,1\,n)} + f_{s(1\,1\,n)}]\, dx\, dy\, dz \tag{3}$$