

## Theory of quantum-wire formation on corrugated surfaces

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One of the possible transformations of an unstable surface is faceting, where the surface rearranges into a hill-and-valley structure in order to decrease its free energy. It was shown by Marchenko (Zh. Eksp. Teor. Fiz. **81**, 1141 (1981) [Sov. Phys. JETP **54**, 605 (1981)]) that the surface faceting of a homogeneous crystal results in a periodic corrugation of the surface. A heterophase system is considered in the present paper. A macroscopic theory of surface free energy is developed for the case of the heterophase lattice-matched system grown on a periodically corrugated substrate where both the substrate and the deposited material are unstable against faceting. There appears an important contribution of the interface energy into the total surface free energy of the heterophase system. It is shown that if the deposited material wets the corrugated substrate, then the homogeneous coverage of the periodically corrugated substrate occurs. If the deposited material does not wet the substrate, then isolated clusters are formed in grooves of the periodically corrugated substrate after the deposition of the first monolayer. The nonwetting situation occurs in a practical case of GaAs/AlAs systems. We compare surface free energies of two heterophase systems. One is a system with homogeneous coverage of a periodically corrugated substrate, and the other is a system with clusters on a periodically corrugated substrate. The competition of surface free energies of the two systems is governed by the interplay of two contributions, namely, of the interface energy  $E_{\text{inter}}$  and the energy  $E_{\text{edges}} + E_{\text{elastic}}$ , where  $E_{\text{edges}}$  is the energy of edges and  $E_{\text{elastic}}$  is the elastic energy. The interface energy is determined by the interface area. The energy  $E_{\text{edges}} + E_{\text{elastic}}$  is determined by the shape of the surface and is minimum for a surface with periodic surface corrugation. There exists then a gain in the interface energy due to the smaller interface area for a two-phase system with clusters with respect to the system with homogeneous coverage. On the other hand, there exists a loss in the energy  $E_{\text{edges}} + E_{\text{elastic}}$  for an aperiodic system with clusters compared to the periodic system with homogeneous coverage. The gain in the interface energy is larger than the loss in the energy  $E_{\text{edges}} + E_{\text{elastic}}$ . This promotes formation of isolated GaAs clusters in grooves of the corrugated AlAs substrate. This result explains the direct fabrication of nanometer-scale quantum-well-wire superlattices on corrugated substrates.

### I. INTRODUCTION

Equilibrium faceting is a phenomenon in which a planar crystal surface rearranges into a periodic hill-and-valley structure with an increased surface area. The faceting is caused by the decrease of the total surface free energy.<sup>1</sup> It is known from experiments that a large number of very different surfaces undergo equilibrium faceting. The most studied surfaces are vicinals to Si(111).<sup>2-5</sup> (The detailed review is given by Williams *et al.*<sup>6</sup>) The faceting was also observed on vicinals to GaAs(100),<sup>7,8</sup> Pt(100),<sup>9</sup> on low-index singular surfaces

Ir(110),<sup>10</sup> TaC(110),<sup>11</sup> on non-(100)-oriented GaAs,<sup>12,13</sup> etc.

Another class of faceted surfaces is associated with the formation of coherent strained islands at initial stages of the heterophase growth on lattice-mismatched substrates. Coherent strained islands were observed in a Ge/Si(001) system,<sup>14,15</sup> in a  $\text{In}_{1-x}\text{Ga}_x\text{As}/\text{GaAs}(001)$  system,<sup>16,17</sup> and in a  $\text{InAs}/\text{GaAs}(001)$  system.<sup>17-19</sup> The growth of coherent strained islands was theoretically explained by the instability of planar surfaces in stressed systems.<sup>20-23</sup> The top surface of a coherent strained island is faceted due to the gain in the strain energy, which

exceeds the loss in the surface free energy. The gain in the strain energy makes coherent strained islands more favorable with respect to both uniformly strained films and dislocated islands<sup>23</sup> and may lead to an ordered array of coherent islands.<sup>24</sup>

The effect of externally applied stress on the faceting, which initially occurs *without* any external stress, is studied in Ref. 25 for a heterophase system where an epitaxial film is coherently grown on a lattice-mismatched *planar* substrate. It was shown that applying an external stress, which is below a certain critical value, results in controlled tuning of the period of a faceted structure. If the external stress exceeds the critical value, the faceting vanishes.

Recent interest in surface faceting and other related phenomena is stimulated by the possibilities of the direct fabrication of ordered arrays of quantum wires and quantum dots with interesting physical properties and device applications.<sup>26</sup>

In the present paper we consider the heterophase system, where an epitaxial film is being grown coherently on a faceted, or corrugated, substrate. We study the transformation of the faceted surface structure as the result of the heteroepitaxial growth. The treatment is focused on the quasiequilibrium growth, where the crystal surface tends to come to the configuration, which corresponds to the minimum of the free energy. Concerning the question whether the growth is close to an equilibrium growth or not, we may compare two characteristic time intervals. The first is the time  $\Delta t_{\text{eq}}$ , which is needed to bring the surface to the equilibrium configuration by means of the migration of surface atoms. The second is the time  $\Delta t_{\text{dep}}$  required for the deposition of 1 ML. At low growth rates where

$$\Delta t_{\text{eq}} \ll \Delta t_{\text{dep}},$$

the migration kinetics are sufficiently fast in order to bring the surface to equilibrium. The shape of the surface is then determined by the minimum of the free energy.

The Helmholtz free energy of a faceted surface was studied by Marchenko.<sup>27</sup> It was shown that the surface free energy consists of three terms:

$$F = E_{\text{facets}} + E_{\text{edges}} + E_{\text{elastic}}, \quad (1)$$

$E_{\text{facets}}$  being the free energy of facet planes,  $E_{\text{edges}}$  being the short-range energy of facet edges, and  $E_{\text{elastic}}$  being the elastic energy associated with the edges. Equation (1) is valid for a macroscopic faceting, which should be distinguished from a microscopic surface reconstruction. (The latter is not considered here.) The facet is well defined if its characteristic width  $L_F$  is much larger than the lattice constant  $a$ . We focus in the present paper on the macroscopic faceting where  $L_F \gg a$ . For vicinal surfaces, a more severe restriction reads that the width of the facet must be much larger than the terrace width.

The first term on the right-hand side of Eq. (1),  $E_{\text{facets}}$ , is proportional to the surface area, whereas the second and the third terms are associated with edges and are less than  $E_{\text{facets}}$  due to the small parameter  $a/L_F \ll 1$ . The energy  $E_{\text{facets}}$  was studied in detail by Herring,<sup>1</sup>

Wulff,<sup>28</sup> and Rottman and Wortis.<sup>29</sup> The equilibrium crystal shape is determined by the Wulff construction,<sup>28</sup> which implies the minimum of the free energy of all facets under the constraint of the constant volume of the crystal. We use here the formulation of the problem, more relevant to the experimental situation where only the top surface of a crystal is studied. It requires additional constraints of fixed bottom and side surfaces and of a fixed "average" normal to the upper surface. If the top surface breaks up into facets, the free energy of all facets, defined per unit area of the reference flat surface with the normal  $\hat{\mathbf{n}}$ , is equal to<sup>1,29</sup>

$$E_{\text{facets}} = \frac{1}{S} \int \frac{\varepsilon(\hat{\mathbf{m}})}{\hat{\mathbf{m}} \cdot \hat{\mathbf{n}}} dS. \quad (2)$$

Here  $\varepsilon(\hat{\mathbf{m}})$  is the free energy per unit area of the surface with the orientation of the normal  $\hat{\mathbf{m}}$ , and  $S$  is the total area of the reference flat surface. The free energy (2) should be minimized under the constraint

$$\frac{1}{S} \int \hat{\mathbf{m}} dS = \hat{\mathbf{n}}. \quad (3)$$

When the upper surface of a crystal breaks up into facets, there appear either sharp crystal edges or narrow rounded parts of the surface at the intersections of neighboring facets. Both types of intersections may be described as linear defects. These linear defects give a short-range contribution into the surface free energy, which is proportional to the length of defects, and a long-range contribution due to elastic strain energy. We focus on the case of sharp edges. Macroscopic treatment is possible also for rounded intersections between facets.

Let us specify energies  $E_{\text{edges}}$  and  $E_{\text{elastic}}$  for the particular case of faceted structures that we study in the present paper. We consider the situation where the minimum of the free energy of facets (2) under the constraint (3) is attained for a one-dimensional symmetric array of facets shown in Fig. 1,  $\varphi$  being the tilt angle of facets. Small energy terms  $E_{\text{edges}} + E_{\text{elastic}}$  do not affect the tilt angle  $\varphi$ . However, it was shown by Marchenko<sup>27</sup> that the minimum of the free energy (1) where both  $E_{\text{edges}}$  and  $E_{\text{elastic}}$  are taken into account, corresponds to the periodic array of facets. The energies  $E_{\text{edges}}$  and  $E_{\text{elastic}}$  depend on the period  $L$ , and the interplay of these energies determines the optimum period of surface corrugation.

There are two types of crystal edges for a faceted surface displayed in Fig. 1, namely, convex and concave edges. Let us denote energies of these edges per unit length of an edge  $\eta^+(\varphi)$  and  $\eta^-(\varphi)$ , respectively. Then the energy of edges per unit area of the reference flat surface is equal to

$$E_{\text{edges}} = \frac{\eta^+(\varphi) + \eta^-(\varphi)}{L}. \quad (4)$$

Elastic energy in the system with the corrugated surface occurs due to the intrinsic surface stress (or the surface tension of the solid). The elastic strain energy of the system defined per unit area of the reference flat surface is then equal to<sup>30</sup>

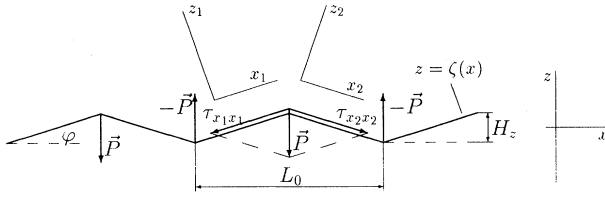


FIG. 1. Effective elastic forces at crystal edges. The tensor of the intrinsic surface stress  $\tau_{ij}$  is defined in local systems of coordinates  $(x_1, y, z_1)$  and  $(x_2, y, z_2)$ . For a symmetric sawtooth profile,  $\tau_{x_1 x_1} = \tau_{x_2 x_2} = \tau$ ;  $P_x = 0$ ,  $P_z = \pm 2\tau \sin \varphi$ . Here  $\zeta(x)$  is the profile of surface corrugation,  $L_0$  is the period of corrugation, and  $H_z$  is the height of corrugation.

$$E_{\text{elastic}} = \frac{1}{2S} \int \sigma_{ij}(\mathbf{r}) u_{ij}(\mathbf{r}) dV + \frac{1}{S} \int \tau_{ij}(\mathbf{r}) u_{ij}(\mathbf{r}) dS. \quad (5)$$

Here  $u_{ij}(\mathbf{r})$  is the strain tensor, and  $\sigma_{ij}(\mathbf{r})$  is the stress tensor, and  $\tau_{ij}(\mathbf{r})$  is the intrinsic surface stress tensor. The intrinsic surface stress tensor  $\tau_{ij}$  depends on the orientation of the facet. It has nonzero components  $\tau_{ij}$  in the facet plane, and the other components vanish. The tensor  $\tau_{ij}$  is constant along the given facet and has discontinuities at crystal edges separating neighboring facets. The discontinuity of the tensor  $\tau_{ij}$  is the source of the strain field in the crystal with corrugated surface. The elastic energy of Eq. (5) may be reduced to the form where these sources appear explicitly:<sup>27</sup>  $E_{\text{elastic}} = -(2S)^{-1} \int u_i(\mathbf{r}) \nabla_\beta \tau_{i\beta}(\mathbf{r}) dS$ ,  $\mathbf{u}_i(\mathbf{r})$  being the displacement vector and  $\beta$  being the two-dimensional index in the local facet plane. The sources of the strain field for the particular faceted structure displayed in Fig. 1 may be described as effective elastic forces  $\mathbf{P}$  applied to crystal edges

$$P_i(x, \zeta(x)) = \pm 2\tau \sin \varphi \delta_{iz} \delta(x - x_n), \quad (6)$$

where  $\zeta(x)$  is the profile of the faceted surface,  $x_n$  is the location of the  $n$ th edge, and  $\tau$  is the component of the intrinsic surface stress tensor  $\tau_{ij}$  defined in Fig. 1.

It should be noted that the strain field also occurs in the case of a planar surface. Elastic relaxation near the planar surface results in static displacements of atoms from their bulk positions. These displacements decay exponentially at a depth of a few lattice constants.<sup>31</sup> The same is also valid for static displacements of atoms caused by microscopic surface reconstruction (see, e.g., Ref. 32). The contributions into the surface free energy caused by both relaxation and reconstruction of planar surface are included into the macroscopic quantity  $\varepsilon(\hat{\mathbf{m}})$ , which enters Eq. (2).

Contrary to this, effective elastic forces  $P_i$  from Eq. (6) create a long-range strain field. Static displacements of atoms from their bulk positions decay inside the crystal at a macroscopic depth, which is equal by an order of magnitude to the period  $L$  of the faceted structure.

The elastic strain energy  $E_{\text{elastic}}$  in the case of small

tilt angle  $\varphi$  of facets was calculated in Ref. 27 by means of the continuum theory of elasticity in the approximation of elastically isotropic medium. It is given in terms of the intrinsic surface stress  $\tau$ , Young's modulus  $Y$ , and Poisson's ratio  $\nu$  as follows:

$$E_{\text{elastic}}(L) = - \frac{8(1-\nu^2)\tau^2\varphi^2}{\pi Y L} \ln \left( \frac{L}{2\pi a} \right), \quad (7)$$

$a$  being a microscopic cutoff length, introduced via Lorentzian broadening of the force density of Eq. (6). This microscopic cutoff length is of the same order of magnitude as the lattice constant. For simplicity, we assume that the cutoff parameter is exactly the lattice constant  $a$ . The logarithmic dependence of the elastic energy on  $L$  is a general feature of any linear defect. It remains in the case of rounded edges, too. For large tilt angles  $\varphi$ , the energy  $E_{\text{elastic}}$  may be calculated numerically.

Summing contributions of Eqs. (2), (4), and (7), we may write down the total surface free energy as follows:

$$F = \frac{\varepsilon(\varphi)}{\cos \varphi} + \frac{C_1(\varphi)}{L} - \frac{C_2(\varphi)}{L} \ln \left( \frac{L}{2\pi a} \right). \quad (8)$$

Here  $C_1(\varphi) = \eta^+(\varphi) + \eta^-(\varphi)$ ,  $C_2(\varphi) = 8(1-\nu^2)g(\varphi;\nu)\tau^2(\varphi)\varphi^2/(\pi Y)$ , and the factor  $g(\varphi;\nu)$  is a numerical factor dependent on the angle  $\varphi$ ,  $g(0;\nu) = 1$ . The energy (8) attains minimum value at

$$L_0 = 2\pi a \exp \left[ \frac{C_1(\varphi)}{C_2(\varphi)} + 1 \right]. \quad (9)$$

The functions  $C_1(\varphi)$  and  $C_2(\varphi)$ , which enter Eqs. (8) and (9), may be found in an explicit form in the limit of small tilt angles  $\varphi$ . If the reference flat surface ( $\varphi = 0$ ) is a low-index singular crystal surface, then facets are vicinals, and the edge between neighboring facets is the place where a sequence of mounting steps is changed by a sequence of descending steps. The energy of the edge is then proportional to the characteristic energy of the interaction between neighboring steps. The latter depends on the distance between steps (i.e., on the terrace width  $L_T$ ) as  $(a/L_T)^2 \sim \varphi^2$ .<sup>30</sup> This implies that energies of edges are equal to  $\eta^+(\varphi) = \xi^+\varphi^2$ ,  $\eta^-(\varphi) = \xi^-\varphi^2$ , and  $\eta(\varphi) = \eta^+(\varphi) + \eta^-(\varphi) = (\xi^+ + \xi^-)\varphi^2$ , where  $\xi^+$ ,  $\xi^-$  do not depend on  $\varphi$ . Therefore, both constants  $C_1(\varphi)$  and  $C_2(\varphi)$  entering Eqs. (8) and (9) are proportional to  $\varphi^2$  at small  $\varphi$ , and the optimum period  $L_0$  from Eq. (9) is  $\varphi$  independent as  $\varphi \rightarrow 0$ .

The periodically corrugated surface with the period  $L_0$  is the configuration with the lowest surface energy. It describes the shape of the surface at temperature  $T = 0$ . Deviations from periodic corrugation, which occur at finite temperatures, and the role of entropy contributions to the free energy are considered in Sec. II. It is shown that the role of entropy effects in the case of a faceted surface is considerably less than in the case of a stepped vicinal surface. The free energy of the surface is then approximately equal to the energy of the surface. Therefore, we do not take into account entropy effects in the remainder of the paper and focus on the calculation of

the surface energy.

In Sec. III, we study distinct heterophase structures on periodically corrugated substrates and compare their energies. We focus on the situation where both the substrate surface and the surface of the deposited material are unstable against faceting. To obtain energies in an analytic form, we consider faceted surfaces with small tilt angles  $\varphi$  of facets. We show that the selection between possible heterophase structures is governed by the fact of whether the deposited material *wets or does not wet* the substrate. In the wetting case, the homogeneous coverage of the periodically corrugated substrate is shown to occur, and the deposited material reproduces the shape of the faceted substrate. In the nonwetting case, clusters of the deposited material appear on a periodically corrugated substrate. The periodic surface corrugation is restored after the deposition of the first several monolayers. Then the hills of the top surface of the heterophase system appear over the valleys of the substrate and vice versa. Thus, a continuous layer of the deposited material with periodically modulated thickness is formed.

In Sec. IV, we apply our general approach to the particular heterophase system GaAs/AlAs(311) where both the growth of GaAs on AlAs and vice versa result in formation of isolated clusters after the deposition of the first monolayer and lead to the formation of a layer with periodically modulated thickness after the deposition of 6 ML.<sup>12,13,33</sup> Although the values of surface energies and intrinsic surface stresses of facets are not known for the system in question, we consider these quantities as macroscopic parameters. We show that the experimental data of Refs. 12, 13, and 33 may be explained if one assumes that the difference of surface energies of tilted (311) facets of GaAs and AlAs is very small. For this case, we compare surface energies of two heterophase systems. One is the system with homogeneous coverage of the periodically corrugated substrate, and the other is a system with clusters on the periodically corrugated substrate. The competition of surface energies of the two heterophase systems is governed by the interplay of two contributions, namely, of the interface energy  $E_{\text{inter}}$  and the energy  $E_{\text{edges}} + E_{\text{elastic}}$ . The interface energy is determined by the interface area. The energy  $E_{\text{edges}} + E_{\text{elastic}}$  is determined by the shape of the surface and is minimum for the surface with periodic surface corrugation.

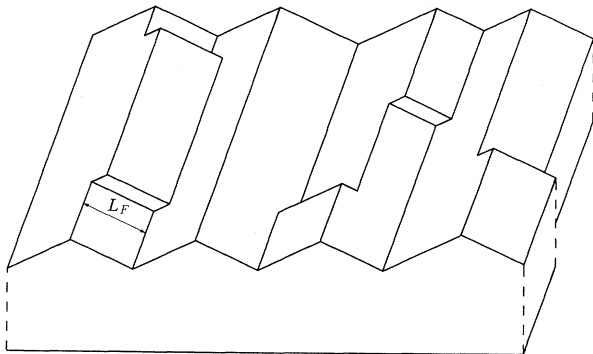


FIG. 2. Low-energy steps on faceted surface;  $L_F$  being the facet width.

There exists then a gain in the interface energy due to the smaller interface area for a two-phase system with clusters compared to the system with homogeneous coverage. On the other hand, there exists a loss in the energy  $E_{\text{edges}} + E_{\text{elastic}}$  for an aperiodic system with clusters compared to the periodic system with homogeneous coverage. The gain in the interface energy is larger than the loss in the energy  $E_{\text{edges}} + E_{\text{elastic}}$ . This promotes formation of isolated clusters during the deposition of the first monolayer of GaAs on the AlAs(311) periodically corrugated surface. This result explains the direct fabrication of nanometer-scale quantum-well-wire superlattices on corrugated substrates.

Section V contains conclusions to the paper.

## II. ENTROPY EFFECTS IN EQUILIBRIUM FACETING

At finite temperatures  $T$ , the surface deviates from ideal corrugation. The analysis of these deviations is simpler for facets that are low-index ones and not vicinal ones. [An example is TaC where the (110) surface breaks up into (100) and (010) facets.<sup>11</sup>] Then, if the temperature  $T$  is far below the roughening transition temperature of facets  $T_R$ , only low-energy configurations of the shape of the surface occur. These configurations contain short steps running across facets from a convex edge to a concave edge (Fig. 2). The energy of this step is  $\lambda_S L_F$ , where  $\lambda_S$  is the step energy per unit length and  $L_F$  is the facet width. Each step shifts (by one lattice constant) positions of convex and concave edges bounding the given facet. This yields the effective meandering of edges.

Thus, there exists a certain analogy between a faceted surface with meandering edges and a vicinal surface with meandering steps. A step on a facet corresponds to a kink on a step on a vicinal surface. One should note, however, important differences between these two systems.

(1) The energy of a step on a facet is approximately  $N_F$  times larger than the energy of a single kink. ( $N_F$  being the number of lattice constants across the facet.) To estimate the average spacing between steps on a facet, one may use the corresponding expression from Ref. 34 for the spacing between kinks on a step and substitute there, instead of the energy of a single kink, the large energy  $\lambda_S L_F$  of a step running across the facet. Then the average spacing between steps on facets, equal to  $l_S \approx a \exp(\lambda_S L_F / T)$ , is much larger than the average spacing between kinks on a given step on a vicinal surface. Steps on facets introduce thus only large-scale roughness, which implies the distribution of facet widths.

(2) Long-range elastic stresses result in effective energetic repulsion between neighboring convex and concave edges, in addition to entropic repulsion. The energetic repulsion between neighboring edges of a faceted surface is the monopole-monopole elastic repulsion [ $U(x) \sim -\ln x$ ], which is much stronger than the dipole-dipole elastic repulsion [ $U(x) \sim 1/x^2$ ], Ref. 30 between steps on a vicinal surface. Entropic repulsion is basically the same in both cases. The total repulsion for a faceted surface is

therefore stronger, and it reduces the probability of small facet widths. The observed distribution of facet widths<sup>11</sup> is half as narrow as the distribution of terrace widths known for vicinal surfaces.<sup>5,35</sup>

The detailed study of facet width distribution and finite-temperature corrections to the free energy of a faceted surface will be presented elsewhere. Below we focus on heterophase structures where an epitaxial growth is being performed on a faceted surface. For these purposes, it is sufficient to consider the substrate as a periodically corrugated one. In our treatment, we will not distinguish the energy and the free energy of the system and we will search the minimum of the energy of the heterophase system.

### III. ENERGY OF A HETEROEPITAXIAL SYSTEM ON A FACETED SUBSTRATE

The surface energy of a heteroepitaxial system where material 2 is being grown on a faceted substrate 1 is as follows:

$$E = E_{\text{facets}} + E_{\text{interface}} + E_{\text{edges}} + E_{\text{elastic}}. \quad (10)$$

We start the discussion of the energy terms of Eq. (10) with the energy of facets  $E_{\text{facets}}$ , which was the major contribution to the surface energy of a homogeneous system. If the planar surface with the orientation  $\hat{n}_0$  is a stable surface of material 2, then the first term in Eq. (10) exhibits the tendency to planarization. We study here the opposite situation where both material 2 of the growing film and substrate 1 are unstable against faceting.

Concerning the elastic strain energy  $E_{\text{elastic}}$ , the following note should be given. There are two sources of the strain field in a heterophase system, namely, effective elastic forces  $\mathbf{P}$  acting at crystal edges and the lattice mismatch ( $\Delta a/a$ ). The contribution of these two sources into the energy of the system, which undergoes surface faceting, was considered in Ref. 25 for the heteroepitaxial lattice-mismatched growth on a *planar* substrate. The results of Ref. 25, which are qualitatively applicable also in our case, read that the surface-stress-induced strain is the dominant one if

$$\left| \frac{\Delta a}{a} \right| \frac{Y L_0}{2\tau} \lesssim 1. \quad (11)$$

Substituting  $Y \sim 500 \text{ meV}/\text{\AA}^3$ ,  $\tau \sim 100 \text{ meV}/\text{\AA}^2$ , and  $L_0 \approx 30 \text{ \AA}$ , the estimate yields  $|\Delta a/a| \lesssim 1.3\%$ . Below we study the case where conditions (11) are satisfied, and we neglect mismatch-induced strain.

We focus here on the particular situation where both materials 1 and 2 tend to form faceted structures, facets being tilted at the same angle  $\varphi_0$  to the reference flat surface, and both structures having the same period  $L_0$ . A practical example of such a system [the GaAs/AlAs(311) heterophase system] will be considered in detail below, in Sec. IV. Then, the energy of facets  $E_{\text{facets}}$  [the first term in Eq. (10)] remains the major contribution to the total surface energy  $E$  of the heterophase system. We

consider below only those heterophase systems where all facets are tilted by the angle  $\pm\varphi_0$ , and  $E_{\text{facets}}$  attains its minimum value. Material 2 deposited onto a faceted substrate 1 may form either a homogeneous coverage or clusters. Distinct heterophase structures are shown in Fig. 3. Figure 3(a) displays the case of homogeneous coverage of the periodically corrugated substrate. It corresponds to the amount  $\Theta$  of the deposited material 2, where  $\Theta > 1 \text{ ML}$ . The periodic corrugation of the top surface of the heterophase structure persists in this case.

Figure 3(b) displays the heterophase system where isolated clusters of material 2 fill locally the entire depth of grooves in some places of substrate 1, whereas grooves remain empty on the rest of the substrate. The typical view of this heterophase system is presented in Fig. 4. The periodic corrugation of the surface disappears in this case due to clusters. The substrate 1 is covered only partially as long as the amount  $\Theta$  of the deposited material 2 is  $\Theta < N_Z$ . ( $N_Z$  being the height of the surface corrugation, defined in units of the monolayer height.) If the amount  $\Theta$  of the deposited material 2 is  $\Theta \geq N_Z$ , the periodic corrugation of the surface with the period  $L_0$  is recovered. Then the hills of the top surface of the heterophase system appear over the valleys of the substrate and vice versa. Thus, a continuous layer of the deposited material with periodically modulated thickness is formed [Fig. 3(d)].

Figure 3(c) displays the heterophase system with “thin” clusters of material 2, the clusters being formed in all grooves of the corrugated substrate 1. The periodic corrugation of the surface persists in this case but the particular shape of the surface is different from the substrate shape due to clusters. If the amount  $\Theta$  of the

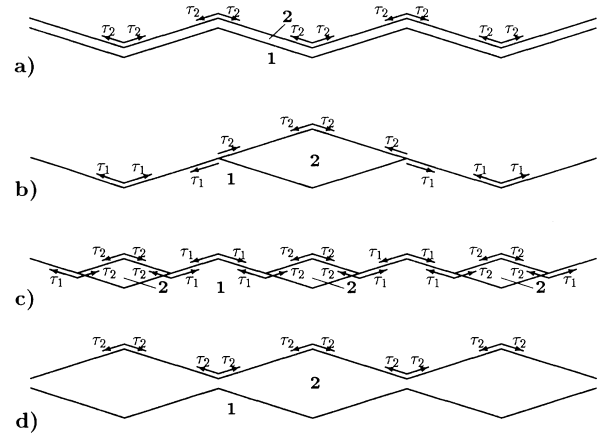


FIG. 3. Distinct structures of the heterophase system and effective elastic forces. (a) Homogeneous coverage  $\Theta > 1$ ; (b) System with separated thick clusters; (c) System of thin clusters; (d) Heterophase system at high coverage  $\Theta \geq N_Z$ , where the periodic surface corrugation is restored, and the hills of the top surface of the heterophase system appear over the valleys of the substrate and vice versa. The heterophase system contains a continuous layer of material 2 with periodically modulated thickness.

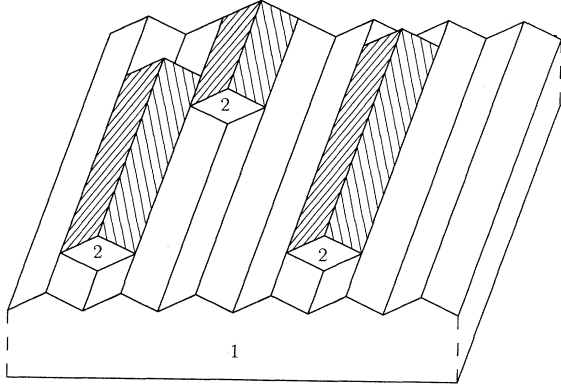


FIG. 4. Clusters in the heterophase system on a periodically corrugated surface.

deposited material 2 is  $\Theta \geq N_Z$ , the surface of material 2 exhibits the configuration of Fig. 3(d).

In order to find the criterion of formation of each of the heterophase systems displayed in Fig. 3, we have to make certain assumptions about the growth kinetics. During the deposition of the first monolayer of material 2, deposited atoms migrate in order to decrease the total energy of the system. There exist two characteristic time intervals. The first is the time interval  $\Delta t_{\text{eq}}$ , which is needed to bring the surface to the equilibrium configuration by means of the migration of surface atoms. The second is the time interval  $\Delta t_{\text{dep}}$  required for the deposition of 1 ML. At low growth rates where

$$\Delta t_{\text{eq}} \ll \Delta t_{\text{dep}}, \quad (12)$$

the migration kinetics are sufficiently fast in order to bring the surface to the equilibrium configuration corresponding to the minimum of the surface energy. The selection between the homogeneous coverage [Fig. 3(a)] and the formation of clusters [Figs. 3(b) or 3(c)] occur during the deposition of the first monolayer. Then, if the system with fractional monolayer coverage is energetically favorable, the further deposition will result in the completion of the monolayer and in the continuous growth of the periodically corrugated heterophase structure of Fig. 3(a). If the system of separated thick clusters [displayed in Fig. 3(b)] is favorable, the further deposition will lead to formation of new clusters and to elongation of existing ones until they fill all the grooves at the coverage  $\Theta = N_Z$ . If the system of thin clusters [shown in Fig. 3(c)] is favorable, the further deposition will result in the expansion of clusters until they fill all the grooves at the coverage  $\Theta = N_Z$ .

It should be noted that a homogeneous coverage of substrate 1 may lead to the formation of stripes if the amount of the deposited material 2 is less than 1 ML ( $\Theta < 1$ ). Striped patterns were observed, e.g., in heterophase systems  $O/\text{Cu}(110)$ ,<sup>36</sup>  $\text{InAs}/\text{GaAs}(100)$  Ref. 37 with submonolayer coverages of planar substrates. The stripe formation was explained theoretically in Refs. 38–42. It is caused by effective elastic forces acting at steps between two materials. Such a mechanism exists *only* in the case

of submonolayer coverage; it vanishes if the monolayer is completed. We do not consider here the case of a submonolayer coverage  $\Theta < 1$ .

To find the criterion that determines the growth mode occurring on a faceted substrate, we will calculate the energy of all structures shown in Figs. 3(a)–(c) for the amount of the deposited material  $\Theta$  equal to 1 ML.

The energies  $E_{\text{facets}}$ ,  $E_{\text{interface}}$ , and  $E_{\text{edges}}$  in Eq. (10) may be found by calculating areas of facets and interfaces and the number of edges. Although we neglect the small lattice mismatch between materials 1 and 2, we consider the difference between these two materials in the following sense. We take into account a possible difference in energies of facets,  $\varepsilon_2(\varphi_0) - \varepsilon_1(\varphi_0)$ , and a difference in values of the intrinsic surface stress,  $\tau_2 - \tau_1$ . The former governs effects of wetting or nonwetting in the heterophase growth. The latter gives an additional contribution to the elastic strain energy, besides the contribution caused by effective elastic forces at edges. On the other hand, we neglect the difference in values of Young's moduli  $Y$  as well as in values of Poisson's ratios  $\nu$ , which does not lead to any principal effect.

To make an analytic calculation of  $E_{\text{elastic}}$  possible, we consider here a faceted surface with a small tilt angle of facets  $\varphi_0 \ll 1$ . Then  $E_{\text{elastic}}$  may be expressed in terms of effective elastic forces as follows:

$$E_{\text{elastic}} = -\frac{1}{2L_x L_y} \int dx \int dx' \int dy \int dy' P_i(x, y) \times G_{ij}(x - x', y - y') P_j(x', y'), \quad (13)$$

$G_{ij}(x - x'; y - y')$  being the surface Green's tensor of the equilibrium equations of the theory of elasticity,  $L_x$ ,  $L_y$  being the dimensions of the substrate projected onto a reference flat surface. The Green's tensor for elastically isotropic medium is given, e.g., in Ref. 43.

Effective elastic forces  $P_i(x, y)$ , which are the sources of the strain field, are displayed in Figs. 3(a)–(d). Note that, besides forces  $P_z = \pm 2\tau \sin \varphi_0 \approx \pm 2\tau \varphi_0$  acting at crystal edges, there appear forces  $P_x = \pm(\tau_2 - \tau_1) \cos \varphi_0 \approx \pm(\tau_2 - \tau_1)$  acting at interphase line boundaries on the surface.<sup>38,39</sup>

Let us first discuss the energy of a heterophase system with the homogeneous coverage  $\Theta > 1$  (Fig. 3a). The surface energy is then equal to

$$E_1 = +[\varepsilon_2(\varphi_0) + \gamma_{12}(\varphi_0) - \varepsilon_1(\varphi_0)] \left(1 + \frac{\varphi_0^2}{2}\right) - \frac{8(1 - \nu^2)\tau_2^2 \varphi_0^2}{\pi Y L_0}. \quad (14)$$

Here  $\varepsilon_1(\varphi_0)$ ,  $\varepsilon_2(\varphi_0)$  are the surface energies of materials 1 and 2, respectively, energies being defined per unit surface area, and  $\gamma_{12}(\varphi_0)$  is the interface energy per unit interface area. The energies  $\varepsilon_{1,2}(\varphi_0)$  are not expanded in powers of the small angle  $\varphi_0$  because they might have cusps at  $\varphi = \varphi_0$ .

Figure 3(b) displays a heterophase system with thick clusters. If the coverage is equal to  $\Theta \leq N_Z$ , only the fraction  $\bar{q} = \Theta/N_Z$  of the faceted substrate is covered by clusters. Effective elastic forces creating the strain field in the system are shown for the particular positions of

clusters in Fig. 3(b). To find the energy  $E_{\text{elastic}}$  it is necessary to describe effective elastic forces for an arbitrary distribution of clusters. We define the quantity  $q_n(y)$ , which is equal to 1 if the  $n$ th groove of the substrate is covered by a cluster at the point  $y$ , and is equal to 0 otherwise. Then the density of effective elastic forces may be expressed in terms of  $q_n(y)$  as follows:

$$P_x(x, y) = (\tau_2 - \tau_1) \sum_n \left\{ \delta \left[ x - \left( n - \frac{1}{2} \right) L_0 \right] - \delta \left[ x - \left( n + \frac{1}{2} \right) L_0 \right] \right\} q_n(y), \quad (15a)$$

$$P_z(x, y) = \varphi_0 \sum_n \left\{ \tau_1 \left[ -\delta \left[ x - \left( n - \frac{1}{2} \right) L_0 \right] + 2\delta(x - nL_0) - \delta \left[ x - \left( n + \frac{1}{2} \right) L_0 \right] \right] + (\tau_1 + \tau_2) \left[ \delta \left[ x - \left( n - \frac{1}{2} \right) L_0 \right] - 2\delta(x - nL_0) + \delta \left[ x - \left( n + \frac{1}{2} \right) L_0 \right] \right] \right\} q_n(y). \quad (15b)$$

To evaluate the energy  $E_{\text{elastic}}$ , a certain information about distribution of clusters is needed. Expressing  $q_n(y)$  as a sum of the average and fluctuations,

$$q_n(y) = \bar{q} + \delta q_n(y), \quad (16)$$

we may give the following note concerning correlations in fluctuations  $\delta q_n(y)$ . Each cluster with finite length  $l_y$  has front and back surfaces (e.g., front surfaces and marked by the number “2” in Fig. 4). The larger the length of clusters  $l_y$ , the smaller the contribution of front and back surfaces into the total energy of the system. Therefore, only clusters with  $l_y \gg L_0$  are energetically favorable. The correlation function of  $\delta q_n(y)$  may then be written as follows:

$$\langle \delta q_n(y) \delta q_{n'}(y') \rangle = \bar{q}(1 - \bar{q}) K \left( n - n'; \frac{|y - y'|}{L_{\text{corr}}} \right), \quad (17)$$

where the correlation length  $L_{\text{corr}} \gg L_0$ .

Correlations in positions of clusters in a real system depend on kinetics. First clusters are being formed at low coverage  $\Theta < 1$ . Changing the coverage  $\Theta$  results in the change of the minimum energy configuration. Attaining the energy minimum involves rearrangement of matter already assembled in thick clusters with the height  $H_Z > 1$  ML. Time required for such a rearrangement is essentially longer than the required time during the growth of the first monolayer in the case of a homogeneous coverage of Fig. 3(a). The relation (12) between the migration time and the deposition time may be not valid in this case, and the equilibrium distribution of clusters may be not attained. Below we do not search the equilibrium distribution of clusters.

To evaluate the energy of a heterophase system with thick clusters, we will calculate first the energy of a system of uncorrelated clusters. Then, to estimate the effect of correlations, we will calculate the energy for certain particular correlated arrays of clusters.

Let us consider the system where positions of clusters in different grooves are not correlated, and the typical length of a single cluster exceeds  $L_0$ . Then the correlation function reduces to

$$K \left( n - n'; \frac{|y - y'|}{L_{\text{corr}}} \right) = \delta_{n, n'} f \left( \frac{|y - y'|}{L_{\text{corr}}} \right), \quad (18)$$

where  $f(0) = 1$ . Substituting elastic forces  $P_x(x, y)$ ,  $P_z(x, y)$  from Eq. (15) into Eq. (13), and using the correlator of fluctuations  $\langle \delta q_n(y) \delta q_{n'}(y') \rangle$  from Eqs. (17) and (18), we get the surface energy of the heterophase system of Fig. 3(b) as follows:

$$E_2 = \{ \varepsilon_1(\varphi_0) + [\varepsilon_2(\varphi_0) + \gamma_{12}(\varphi_0) - \varepsilon_1(\varphi_0)] \bar{q} \} \left( 1 + \frac{\varphi_0^2}{2} \right) \quad (19a)$$

$$- \frac{8(1 - \nu^2)\varphi_0^2}{\pi Y L_0} [(1 - \bar{q})\tau_1^2 + \bar{q}\tau_2^2] \quad (19b)$$

$$- \bar{q}(1 - \bar{q}) \frac{2(1 - \nu^2)(\tau_2 - \tau_1)^2}{\pi Y L_0} \left[ \ln \frac{L_0}{2\pi a} + \ln \pi \right] \quad (19c)$$

$$+ \frac{\bar{q}(1 - \bar{q})\varphi_0^2}{L_0} \left\{ \frac{2(1 - \nu^2)}{\pi Y} \left[ (\tau_1 + \tau_2)^2 \left( \ln \frac{L_0}{2\pi e a} + \ln \frac{16e}{\pi^3} \right) \right] - (\xi_1^+ + \xi_2^-) \right\}. \quad (19d)$$

The term of Eq. (19a) is the energy of facets and interfaces. This term depends linearly on the fraction of the substrate surface  $\bar{q} = \Theta/N_Z$  covered by material 2. The term of Eq. (19b) is the value of the quantity  $W = E_{\text{edges}} + E_{\text{elastic}}$  evaluated for the periodic corrugation with the period  $L_0$ , material 1 and 2 contributing with factors  $(1 - \bar{q})$  and  $\bar{q}$ , respectively. The term of Eq. (19c) is the negative contribution to  $E_{\text{elastic}}$  due to the difference in values of the intrinsic surface stress between materials 1 and 2. The term of Eq. (19d) is the contribution to the energy  $W = E_{\text{edges}} + E_{\text{elastic}}$  due to

clusters. Since we consider here the case of small tilt angle of facets  $\varphi_0$ , then the term of Eq. (19c) is essentially larger than that of Eq. (19d) [if  $|\tau_2 - \tau_1|$  is not especially small and obeys the relation  $|\tau_2 - \tau_1| \gg (\tau_1 + \tau_2)\varphi_0$ ]. In the particular case where  $\tau_1 = \tau_2 \equiv \tau$ ,  $\xi_2^- = \xi_1^-$ , and  $\xi_2^+ = \xi_1^+$ , the term of Eq. (19c) vanishes, and the term of Eq. (19d) reduces to the positive quantity  $\bar{q}(1 - \bar{q})8(1 - \nu^2)\tau^2\varphi_0^2(\pi Y L_0)^{-1} \ln(16e/\pi^3)$ . The latter means the energy loss in the energy  $W = E_{\text{edges}} + E_{\text{elastic}}$  for an aperiodic system with clusters with respect to the periodically corrugated surface.

To estimate the effect of correlations in positions of clusters on the energy of the heterophase system of Fig. 3(b), we will calculate the energy  $E$  for particular values of the coverage  $\Theta$  where  $\bar{q} \equiv \Theta/N_Z = 1/M$  ( $M$  being an integer number). Then a periodic distribution of clusters is possible where clusters are arranged in a periodic structure and occupy totally 1 of each  $M$  neighboring grooves of the faceted substrate, all the rest

grooves remaining empty. (In reality, this array of clusters at different values of the “ $y$ ” coordinate may be tied to different sets of grooves. Since the typical length of clusters is  $l_y \gg L_0$ , this does not affect the energy of the system.) Correlations in positions of clusters lead to some changes in the energy terms of Eqs. (19c) and (19d). The sum of these terms for a correlated system is equal to

$$-\bar{q} \frac{2(1-\nu^2)(\tau_2-\tau_1)^2}{\pi Y L_0} \left[ \ln \frac{L_0}{2\pi a} + \ln \pi - \ln \frac{\sin(\pi\bar{q})}{\pi\bar{q}} \right] + \frac{\bar{q}\varphi_0^2}{L_0} \left\{ \frac{2(1-\nu^2)}{\pi Y} \left[ (\tau_1+\tau_2)^2 \left( \ln \frac{L_0}{2\pi e a} + \ln \frac{16e}{\pi^3} + \ln \frac{\sin(\pi\bar{q})}{\pi\bar{q}} - 4 \ln \frac{\sin(\pi\bar{q}/2)}{\pi\bar{q}/2} \right) \right] - (\xi_1^+ + \xi_2^-) \right\}. \quad (20)$$

For small values of  $\bar{q} \equiv \Theta/N_Z \ll 1$ , correlations in positions of clusters are not essential, and energies of Eqs. (19) and (20) coincide within the linear approximation in  $\bar{q}$ . The main deviation from the linear approximation at small  $\bar{q}$  occurs due to the factor  $(1-\bar{q})$  in Eqs. (19c) and (19d).

The surface energy of the heterophase system, which contains thin clusters in all the grooves of the faceted substrate [Fig. 3(c)], is equal to

$$E_3 = \left\{ \varepsilon_1(\varphi_0) + [\varepsilon_2(\varphi_0) + \gamma_{12}(\varphi_0) - \varepsilon_1(\varphi_0)] \sqrt{\bar{q}} \right\} \left( 1 + \frac{\varphi_0^2}{2} \right) \quad (21a)$$

$$- \frac{8(1-\nu^2)\varphi_0^2}{\pi Y L_0} \tau_1^2 \quad (21b)$$

$$- \frac{2(1-\nu^2)(\tau_2-\tau_1)^2}{\pi Y L_0} \ln \left[ \frac{L_0}{2\pi a} \sin(\pi r) \right] \quad (21c)$$

$$+ \frac{\varphi_0^2}{L_0} \left( (2\xi_{12}^- - \xi_1^- - \xi_2^-) + \frac{2(1-\nu^2)}{\pi Y} \left\{ (\tau_2-\tau_1)^2 \ln \left( \frac{L_0}{2\pi a} \right) - 4(\tau_2^2 - \tau_1^2) \right. \right. \quad (21d)$$

$$\left. \left. + (\tau_1 + \tau_2) \left[ -4\tau_2 \ln \sin \left( \frac{\pi r}{2} \right) + 4\tau_1 \ln \cos \left( \frac{\pi r}{2} \right) + (\tau_1 + \tau_2) \ln \sin(\pi r) \right] \right\} \right). \quad (21e)$$

Here  $r = \sqrt{\Theta/N_Z}$  is the fraction of the substrate surface covered by material 2. Equation(21) is valid if the widths of all facets of both material 1 and material 2 exceed the lattice constant, i.e., if  $a/(2L_0) \ll r, (1-r)$ . The term of Eq. (21a) includes the energy of facets and interfaces. Equation (21b) represents the value of  $W = E_{\text{edges}} + E_{\text{elastic}}$  for the periodically corrugated surface with the period  $L_0$ . The term of Eq. (21c) is the negative contribution to  $E_{\text{elastic}}$  due to the difference  $(\tau_2 - \tau_1)$ . The terms of Eqs. (21d) and (21e) are contributions to  $W = E_{\text{edges}} + E_{\text{elastic}}$  due to clusters. In the particular case where  $\tau_2 = \tau_1 \equiv \tau$ ,  $\xi_{12}^- = \xi_1^- = \xi_2^-$ , the terms of Eqs. (21d) and (21e) yield the positive contribution to the energy  $8(1-\nu^2)\tau^2\varphi_0^2(\pi Y L_0)^{-1} \ln \{4/[e \sin(\pi r)]\}$ .

It follows from Eqs. (14), (19), and (21) that main contributions to the surface energy for various configurations of the heterophase system comes from the energy of facets and interfaces. These are first terms on the right-hand sides of Eqs. (14), (19), and (21). Other energy terms, namely, the energy of edges and the elastic strain energy are proportional to a small parameter  $a/L_0$ . Comparing the energies  $E_{\text{facets}} + E_{\text{interface}}$  in Eqs. (14), (19), and (21), one comes to the following conclusion. In the *wetting* case where

$$\varepsilon_2(\varphi_0) + \gamma_{12}(\varphi_0) - \varepsilon_1(\varphi_0) < 0, \quad (22)$$

the heterophase system with homogeneous coverage shown in Fig. 3(a) is favorable. The example is the growth of AlAs on periodically corrugated vicinal surface of GaAs(001) 3°-off towards  $[\bar{1}10]$ .<sup>7</sup>

In the *nonwetting* case, where

$$\varepsilon_2(\varphi_0) + \gamma_{12}(\varphi_0) - \varepsilon_1(\varphi_0) > 0, \quad (23)$$

the heterophase system with thick separated clusters displayed in Fig. 3b and in Fig. 4 is favorable. At high coverage,  $\Theta > N_Z$ , the periodic surface corrugation is restored. Then the hills of the top surface of the heterophase system appear over the valleys of the substrate and vice versa. Thus, a continuous layer of the deposited material with periodically modulated thickness is formed. This situation seems to be realized for the growth of GaAs on the vicinal surface of AlAs(001) 3°-off towards  $[\bar{1}10]$ ,<sup>7</sup> and for both GaAs/AlAs and AlAs/GaAs heterophase growth on the (311)*A* surface.<sup>12,13,33</sup>

The heterophase system with thin clusters shown in Fig. 3(c) is not favorable in any case.

The two criteria of Eqs. (22) and (23) allow us to distinguish two principally different situations that may oc-



cur for the heterophase growth. Neither of these criteria contains the value of  $E_{\text{elastic}}$ . Therefore, these criteria, which were derived in the approximation of the small tilt angle of facets,  $\varphi_0 \ll 1$ , are valid in the general case.

If the difference in surface energies  $|\varepsilon_2(\varphi_0) - \varepsilon_1(\varphi_0)|$  exceeds the interface energy  $\gamma_{12}(\varphi_0)$ , then the situation at the heteroepitaxial growth of material 1 on material 2 is opposite to that where material 2 grows on material 1. Let, e.g.,  $\varepsilon_2(\varphi_0) > \varepsilon_1(\varphi_0)$ . Then material 2 does not wet material 1, which promotes formation of separated clusters. On the contrary, it follows from Eq. (22) (indices  $1 \leftrightarrow 2$  being interchanged) that material 1 wets material 2, which promotes homogeneous coverage.

If the difference in surface energies is especially small,

$$|\varepsilon_2(\varphi_0) - \varepsilon_1(\varphi_0)| < \gamma_{12}(\varphi_0), \quad (24)$$

the nonwetting situation may occur both for the growth of material 2 on material 1 and vice versa. Energy terms  $W = E_{\text{edges}} + E_{\text{elastic}}$  may become important in this case. Then the calculation of  $E_{\text{elastic}}$  depends on the actual value of the tilt angle of facets  $\varphi_0$ . This situation will be considered for the particular GaAs/AlAs(311) system in Sec. IV, where  $E_{\text{elastic}}$  will be found numerically for a large tilt angle of facets.

#### IV. FACETING IN THE HETEROPHASE SYSTEM GaAs/AlAs(311)

We consider in Sec. IV an example of the heterophase system grown on a faceted substrate, namely the GaAs/AlAs(311) system. There exist two sets of experimental data concerning the faceting of the GaAs(311)A surface. Experimental data by Nötzel *et al.*<sup>12,13</sup> read that the (311)A surface of GaAs breaks up spontaneously into a one-dimensional array of facets with the lateral periodicity in the  $[01\bar{1}]$  ( $x$ ) direction, the period of surface corrugation  $L_0$  being equal to eight lattice constants,  $L_0 = 8a_x = 8a_{[1\bar{1}0]} = 32 \text{ \AA}$ , and the height of surface corrugation  $H_z$  being equal to six lattice constants,  $H = N_Z a_z = 6a_z = 6a_{[311]} = 10.2 \text{ \AA}$ . According to Ref. 12, the faceted (311)A surface of GaAs consists of alternating  $(3\bar{1}3)$  and  $(33\bar{1})$  facets separated by narrow ( $d = 4 \text{ \AA}$  wide) (311) terraces (Fig. 5). The structure is oriented along the  $[\bar{2}33]$  ( $y$ ) direction.

Alternative experimental data obtained by scanning tunneling microscopy by Wassermeier *et al.*<sup>44</sup> read that the period of the corrugation is  $L_0 = 8a_x = 32 \text{ \AA}$ , whereas the height of the corrugation is  $H = 2a_z = 3.4 \text{ \AA}$ . The reason for this discrepancy is not clear so far. Probably, it may be caused by unintentional misorientation of the substrate with respect to the exact (311)A direction, which is noted in Ref. 13. However, no results on the heterophase growth in the GaAs/AlAs(311) system where the height of the corrugation is 2 ML have been reported up to now, to our knowledge. Therefore, we focus here on the heterophase GaAs/AlAs system in the case where the height of the corrugation is 6 ML.

Experimental data of Refs. 12, 13, and 33 read (i) if AlAs is being deposited on the periodically corrugated

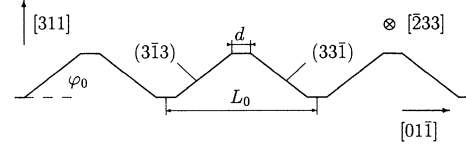


FIG. 5. Schematic view of the faceted GaAs(311)A surface.

GaAs(311) surface (or vice versa), the periodic surface corrugation is restored after the deposition of 6 ML. Then the hills of the top surface of the heterophase system appear over the valleys of the substrate and vice versa. The system of alternating wide and narrow channels of GaAs and AlAs is formed, which is a quantum-well-wire superlattice. (ii) If the amount of deposited GaAs is not sufficient to fill all the grooves on the AlAs surface (and vice versa), then isolated clusters of GaAs are formed. Such clusters of GaAs embedded into the AlAs matrix are isolated quantum wires.

Before applying our consideration of Sec. III to the GaAs/AlAs(311) heterophase system, the following notes should be given:

(1) Since the range of interatomic interactions may exceed one lattice constant, we take into account the possible dependence of the interface energy on the thickness of the epitaxial layer.

(2) It was experimentally proven by Brandt *et al.*<sup>45</sup> that the continuum theory of elasticity predicts correct strains in epitaxial layers on a lattice-mismatched planar substrate if the epilayer thickness is 3 ML or larger. These results encourage us to use the continuum theory of elasticity for the system where the height of surface corrugation is 6 ML.

(3) There exist certain experimental data on the microscopic structure of (331) facets of GaAs and AlAs.<sup>13</sup> However, the existing data are not sufficient to be the basis for microscopic calculations. Some more scanning tunneling microscopy information is necessary, like, e.g., for the case of the corrugated Si(211) surface.<sup>46</sup> Here, following the general approach of the paper, we describe the (331) surfaces of GaAs and AlAs by macroscopic parameters such as the energy of facets  $\varepsilon$  and the intrinsic surface stress  $\tau$ , which, of course, may be different for two materials.

(4) The lattice-mismatch in the GaAs/AlAs heterophase system, equal to approximately 0.04% at typical temperatures of the epitaxy, satisfies the criterion of Eq. (11). Therefore, the mismatch-induced strain is small compared to the surface-stress-induced strain. The former is neglected in our treatment. The GaAs/AlAs system in question is thus considered as a lattice-matched one.

(5) The anisotropy of elastic moduli, which exists in III-V semiconductors, may lead, in certain cases, to principal effects. For example, it was shown by De Caro and Tapfer,<sup>47</sup> that a shear strain appears in epitaxial layers grown on planar low-symmetry lattice-mismatched substrates. The highest value of the shear strain (equal to 40% of the tetragonal deformation) was obtained for

the (311) substrate. However, according to point (4), all components of the mismatch-induced strain tensor are negligibly small for the GaAs/AlAs system in question. As concerns surface-stress-induced strain, both tetragonal deformation  $u_{xx}$ ,  $u_{zz}$ , and shear strain  $u_{xz}$  appear in the plane strain geometry in the approximation of elastically isotropic medium. Therefore, we consider this approximation to be a suitable one for our purposes and use it in the present section.

(6) Narrow (4 Å wide) (311) terraces on the faceted surface of GaAs together with two neighboring edges may be considered as “complex” edges of the faceted surface.

Analyzing experimental data (i) and (ii), we will find relations between energetic parameters of the system, which provide formation of isolated clusters in the heterophase system GaAs/AlAs(311).

We consider the heterophase system (either GaAs/AlAs or vice versa) where  $\Theta = 1$  monolayer of material 2 is deposited on the periodically corrugated substrate of material 1. Let us compare energies of two possible configurations of the heterophase system, namely, the system with a homogeneous monolayer coverage [Fig. 6(a)] and a periodic array of clusters containing one cluster per six periods  $L_0$  [Fig. 6(b)]. For the first structure, the energy is

$$E_{\text{hom}} = \frac{\varepsilon_2(\varphi_0)}{\cos \varphi_0} + E_{\text{inter}}^{\text{hom}} + W_0, \quad (25)$$

where  $W_0$  contains energy terms  $E_{\text{edges}} + E_{\text{elastic}}$  for the periodically corrugated surface. For the second structure, the energy is

$$E_{\text{clus}} = \frac{5 \varepsilon_1(\varphi_0)}{6 \cos \varphi_0} + \frac{1 \varepsilon_2(\varphi_0)}{6 \cos \varphi_0} + E_{\text{inter}}^{\text{clus}} + W_0 + \Delta W, \quad (26)$$

where  $\Delta W$  is the change of the energy  $E_{\text{edges}} + E_{\text{elastic}}$  for the system containing clusters with respect to the periodically corrugated surface with the period of corrugation  $L_0$ .

It follows from experimental data<sup>33</sup> that formation of isolated clusters occurs both for the growth of AlAs on the GaAs(311)A surface and vice versa. This implies that

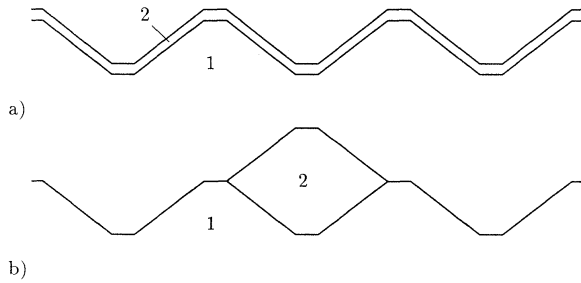


FIG. 6. Possible 1-ML coverages of the (311) faceted surface in the GaAs/AlAs system. (a) Homogeneous monolayer coverage; 1, AlAs, 2, GaAs. (b) Structure with separated GaAs clusters on the AlAs(311) faceted surface; 1, AlAs, 2, GaAs.

the nonwetting situation occurs in both cases. Now we may write the inequality

$$E_{\text{inter}}^{\text{hom}} - E_{\text{inter}}^{\text{clus}} - \frac{5}{6} \frac{|\varepsilon_2(\varphi_0) - \varepsilon_1(\varphi_0)|}{\cos \varphi_0} > \max(\Delta W), \quad (27)$$

which is the sufficient condition of nonwetting both for the growth of material 2 on material 1 and vice versa. If it holds, then the energy of a system with separated clusters given in Eq. (26) is lower than the energy of a system with homogeneous coverage given in Eq. (25).

Now let us check whether the condition of Eq. (27) may hold for reasonable values of parameters.

First, we will evaluate the interface energy. The interface energy in the lattice-matched GaAs/AlAs system is determined by short-range pair interactions of Ga and Al atoms calculated by Wei and Zunger.<sup>48</sup> For the heterophase structures in question,  $E_{\text{interface}}$  is then equal to  $2(\tilde{L}_x a_y)^{-1} \sum_m^M \tilde{\xi}_{2,m} J_{2,m}$ . Here  $\tilde{L}_x = L_0$  for the homogeneous 1-ML coverage and  $\tilde{L}_x = 6L_0$  for the structure with one cluster per six periods  $L_0$ ,  $a_y = 4\sqrt{11}$  Å is the lattice constant in the  $y$  ( $\bar{2}33$ ) direction,  $\tilde{\xi}_{2,m}$  is the number of pairs of Ga and Al atoms separated by the  $m$ th ( $m \leq M = 4$ ) nearest-neighbor distance in the cation sublattice, the numbers of  $\tilde{\xi}_{2,m}$  are defined per one period  $\tilde{L}_x \times a_y$  of the faceted surface. Interaction energies  $J_{2,m}$  are equal to<sup>48</sup>  $J_{2,1} = +0.758$  meV,  $J_{2,2} = -0.089$  meV,  $J_{2,3} = -0.022$  meV, and  $J_{2,4} = -0.112$  meV. The largest “repulsive” term  $J_{2,1}$  determines the positive sign of the interface energy. The coefficients  $\tilde{\xi}_{2,m}$  calculated by counting atoms and the resulting interface energies for the two structures in question are given in Table I. Note that the coefficients  $J_{2,m}$  were calculated in Ref. 48 for interfaces in essentially the bulk GaAs/AlAs heterophase systems. Therefore, applying these numbers is rather accurate for the interface in the system with isolated clusters [displayed in Fig. 6(b)] and less accurate for the system with a homogeneous 1-ML coverage [shown in Fig. 6(a)]. We expect, however, that the model of the interface energy may give a reasonable estimation also for the latter structure.

Thus, the gain in the interface energy of the heterophase AlAs/GaAs structure with separated clusters versus the structure with the homogeneous 1-ML coverage equals

$$E_{\text{inter}}^{\text{hom}} - E_{\text{inter}}^{\text{clus}} = 0.175 \frac{\text{meV}}{\text{Å}^2}. \quad (28)$$

TABLE I. Interface energies of two heterophase GaAs/AlAs structures.

Number of pairs of Ga and Al	$\tilde{\xi}_{2,1}$	$\tilde{\xi}_{2,2}$	$\tilde{\xi}_{2,3}$	$\tilde{\xi}_{2,4}$	$f_{\text{inter}}, \text{meV/Å}^2$
Homogeneous					
1-ML coverage	82	44	166	84	0.212
one cluster per six periods $L_0$	117	87	400	226	0.037

Now let us calculate the difference in the energy  $W = E_{\text{edges}} + E_{\text{elastic}}$  between the structures with homogeneous 1-ML coverage and the structure with one cluster per six periods of corrugation. Note that the contribution to  $E_{\text{edges}}$  for faceted structures in question includes energies of flat narrow (311) terraces and energies of edges themselves. We will describe this energy term by a macroscopic parameter  $\Delta\varepsilon$ . Then the energy  $E_{\text{edges}}$  defined per unit area of the reference flat surface is  $E_{\text{edges}} = \Delta\varepsilon/L$ . To evaluate the sum of energy terms  $W = E_{\text{edges}} + E_{\text{elastic}}$ , it is convenient to use the relation between  $L_0$ ,  $\tau$ , and  $\Delta\varepsilon$  similar to that of Eq. (9). Note that the value of the period  $L = 8a_x = 32 \text{ \AA}$  corresponds to the minimum of the energy  $W = E_{\text{edges}} + E_{\text{elastic}}$  among allowed values of  $L = N_x a_x$ ,  $N_x$  being an integer number. It implies that

$$\begin{aligned} \frac{\Delta\varepsilon}{7a_x} + E_{\text{elastic}}(7a_x) &> \frac{\Delta\varepsilon}{8a_x} + E_{\text{elastic}}(8a_x), \\ \frac{\Delta\varepsilon}{8a_x} + E_{\text{elastic}}(8a_x) &< \frac{\Delta\varepsilon}{9a_x} + E_{\text{elastic}}(9a_x). \end{aligned} \quad (29)$$

To find the allowed interval for the quantity  $\Delta\varepsilon$ , we need values  $E_{\text{elastic}}$  for a set of periods  $L$ . Effective elastic forces acting in the periodically corrugated system in question are displayed in Fig. 7(a). Unlike the difference in the values of  $\tau$  between two materials that yield important negative contribution to  $E_{\text{elastic}}$  in Eqs. (19) and (21), the difference between values  $\tau_1$  and  $\tilde{\tau}_1$  for neighboring facets of the same material makes no principal

effect on  $E_{\text{elastic}}$ . To simplify our treatment we let for each material  $\tilde{\tau}_1 = \tau_1$  and  $\tilde{\tau}_2 = \tau_2$ .

To find  $E_{\text{elastic}}$  as a function of  $L$ , we solve the plane strain problem of the theory of elasticity, that is, we solve the equilibrium equations for the displacement vector  $\mathbf{u}(x; z) = (u_x(x; z); u_z(x; z))$ :

$$(1 - 2\nu)\nabla^2 \mathbf{u}(x; z) + \nabla \text{div} \mathbf{u}(x; z) = 0. \quad (30)$$

Since the structure is periodic and has two mirror planes per each period, we solve Eq. (30) for a half period of periodic structures with different periods  $L$ , applying symmetric boundary conditions (BC) ( $u_x = 0$ ,  $\partial u_z / \partial x = 0$ ) at mirror planes ( $x = 0$  and  $x = L/2$ ) in Fig. 7(a), zero BC in the bulk ( $u_x, u_z \rightarrow 0$  as  $z \rightarrow -\infty$ ), and BC of a stress-free surface ( $\sigma_{ij} \hat{m}_j = 0$ ) everywhere at the upper surface except edges. Solving Eq. (30) by the finite element method<sup>49</sup> yields values of  $E_{\text{elastic}}$  for a set of periods  $L$ . Substituting the values of  $E_{\text{elastic}}$  calculated for  $L = 7a_x$ ,  $L = 8a_x$ , and  $L = 9a_x$  into Eq. (29), we get the following interval for possible values of  $\Delta\varepsilon$ :

$$12.8 \left( \frac{\tau_1}{\tau_0} \right)^2 \frac{\text{meV}}{\text{\AA}} < (\Delta\varepsilon)_1 < 14.6 \left( \frac{\tau_1}{\tau_0} \right)^2 \frac{\text{meV}}{\text{\AA}}, \quad (31)$$

the similar relation being valid also for material 2. The normalization quantity  $\tau_0 = 100 \text{ meV/\AA}^2$  in Eq. (31) is the characteristic value of the intrinsic surface stress.

Now, to find the difference in the energy  $W = E_{\text{edges}} + E_{\text{elastic}}$  between the structure with homogeneous monolayer coverage and the structure containing one cluster per six periods of corrugation, we solve Eq. (30) by the finite element method also for a half period of the heterophase structure with clusters [displayed in Fig. 7(b)]. We assume quantities  $\Delta\varepsilon$  to be equal to the arithmetic mean of two limiting values of the interval in Eq. (31). Finally, we get

$$\begin{aligned} \Delta W &\equiv W^{\text{clus}} - W^{\text{hom}} \\ &= 0.044 \left( \frac{\tau_1}{\tau_0} \right)^2 \frac{\text{meV}}{\text{\AA}^2} - 0.151 \left( \frac{\tau_1}{\tau_0} \right) \left( \frac{\tau_2 - \tau_1}{\tau_0} \right) \frac{\text{meV}}{\text{\AA}^2} \\ &\quad - 0.132 \left( \frac{\tau_2 - \tau_1}{\tau_0} \right)^2 \frac{\text{meV}}{\text{\AA}^2}. \end{aligned} \quad (32)$$

In the particular case where  $\tau_2 = \tau_1$ , the quantity  $\Delta W$  has a positive value  $0.044 \text{ meV/\AA}^2$ . It is the loss in the energy  $E_{\text{edges}} + E_{\text{elastic}}$  for the heterophase system with clusters compared to the heterophase system with homogeneous coverage. If  $\tau_2 \neq \tau_1$ , there appears some negative contribution to  $\Delta W$  proportional to  $(\tau_2 - \tau_1)^2$ , as well as the contribution  $\sim \tau_1(\tau_2 - \tau_1)$ . Contrary to faceted structures with small tilt angle of facets considered in Sec. III, all contributions into  $\Delta W$  for the structure with large tilt angle of facets are of the same order of magnitude.

To check whether the sufficient condition of the non-wetting situation [that of Eq. (27)] holds, we compare  $E_{\text{inter}}^{\text{hom}} - E_{\text{inter}}^{\text{clus}}$  from Eq. (28) and  $\Delta W$  from Eq. (32). Although values of the intrinsic surface stress for (331) facets of GaAs and AlAs are not present in literature, we may use for estimations the values of  $\tau$  for Si(100)  $2 \times 1$  reconstructed surface<sup>39,50,51</sup> and those for GaAs(100)  $2 \times 4$

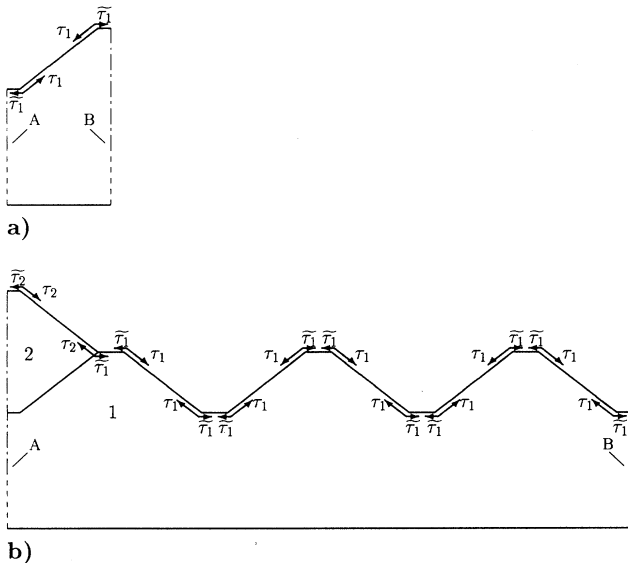


FIG. 7. Effective elastic forces in the faceted heterophase GaAs/AlAs(311) system. (a) Half period of the periodically corrugated structure with the period  $L_0$ ; A and B denote mirror planes  $x = 0$  and  $x = L_0/2$ , respectively. (b) Half period of the heterophase system containing one cluster of GaAs per six periods  $L_0$  of AlAs(311) faceted surface. 1, AlAs, 2, GaAs, A and B denote mirror planes  $x = 0$  and  $x = 3L_0$ , respectively.

reconstructed surface.<sup>52</sup> None of these values exceeds  $\tau_0 = 100 \text{ meV}/\text{\AA}^2$ . It follows then from Eq. (32) that  $\Delta W \leq 0.087 \text{ meV}/\text{\AA}^2$ , i.e.,  $\Delta W$  is less than one half of the gain in the interface energy from Eq. (28). Substituting this value into Eq. (27) we find that if the difference in the energy of the (331) facets between GaAs and AlAs is small enough,  $|\varepsilon_2 - \varepsilon_1| < 0.067 \text{ meV}/\text{\AA}^2$ , then the sufficient condition of the nonwetting [Eq. (27)] holds. This is rather strong restriction on the value  $|\varepsilon_2 - \varepsilon_1|$ . There exist certain possibilities where weaker restrictions on  $|\varepsilon_2 - \varepsilon_1|$  may be sufficient to provide cluster formation both for GaAs/AlAs(311) and for AlAs/GaAs(311) growth. First, if the values of the intrinsic surface stress  $\tau_1$  and  $\tau_2$  are close to each other,  $|\tau_2 - \tau_1| \ll \tau_1$ , Eq. (32) reduces to  $\Delta W = 0.044(\tau_1/\tau_0)^2 \text{ meV}/\text{\AA}^2$ . Second, we may use for the estimation of  $\tau_1$  the maximum value of intrinsic surface stress calculated for GaAs(001)  $2 \times 4$  reconstructed surface, which equals  $66 \text{ meV}/\text{\AA}^2$ .<sup>52</sup> Then the sufficient condition for the formation of clusters [Eq.(27)] reduces to  $|\varepsilon_2 - \varepsilon_1| < 0.145 \text{ meV}/\text{\AA}^2$ . One more possibility to get a weaker restriction on  $|\varepsilon_2 - \varepsilon_1|$  is associated with the above used approach for evaluation of the interface energy. The evaluation of the interface energy for a system with a homogeneous monolayer coverage,  $E_{\text{inter}}^{\text{hom}}$ , by using bulk values of interaction energies between Ga and Al atoms may yield an underestimation of the interface energy. Then the value of the gain in the interface energy,  $E_{\text{inter}}^{\text{hom}} - E_{\text{inter}}^{\text{clus}}$ , may be larger than  $0.175 \text{ meV}/\text{\AA}^2$  calculated in Eq. (28). This again favors formation of clusters.

Summarizing the discussion of the present Section, we make the following remarks. If the sufficient condition for the nonwetting (27) holds, then the gain in the interface energy for a system containing one cluster per six periods of corrugation with respect to the system with the homogeneous monolayer coverage exceeds the loss in the energy  $E_{\text{edges}} + E_{\text{elastic}}$ . This promotes formation of isolated clusters during the deposition of the first monolayer of GaAs on the AlAs(311) periodically corrugated surface. The periodic surface corrugation is restored after the deposition of 6 ML. Then the hills of the top surface of the heterophase system appear over the valleys of the substrate and vice versa. The system of alternating wide and narrow channels of GaAs and AlAs is then formed, which is a quantum-well-wire superlattice.

## V. CONCLUSIONS

We have developed the macroscopic theory of the quasiequilibrium heterophase growth on periodically corrugated substrates. Our approach consists of calculating the energy of the heterophase system. The energy includes the energy of facet planes, interface energy, short-range energy of crystal edges, and elastic strain energy.

We have shown that our macroscopic approach allows us to answer the question of whether the coverage of a corrugated substrate is homogeneous or inhomogeneous.

The selection between two possible growth modes is determined in the macroscopic approach by the fact of whether the deposited material *wets or does not wet* the substrate. If the deposited material wets the substrate, then the homogeneous coverage of the periodically corrugated substrate occurs. The example is the growth of AlAs on the periodically corrugated vicinal surface of GaAs(001)  $3^\circ$  off towards  $[1\bar{1}0]$ .<sup>7</sup>

If the deposited material does not wet the substrate, then isolated clusters of the deposited material appear on the periodically corrugated substrate. This situation seems to be realized for the growth of GaAs on vicinal surface of AlAs(001)  $3^\circ$  off towards  $[1\bar{1}0]$ ,<sup>7</sup> and for both GaAs/AlAs and AlAs/GaAs heterophase growth on the (311)A surface.<sup>12,13,33</sup>

In the case of inhomogeneous cluster coverage, the periodic surface corrugation is restored after the deposition of the first several monolayers. Then, the hills of the top surface of the heterophase system appear over the valleys of the substrate and vice versa, and a continuous layer of the deposited material with periodically modulated thickness is formed. Thus, formation of clusters allows direct fabrication of quantum-well-wire superlattices in heterophase semiconductor systems.

Surface reconstruction on facet planes is taken into account in our theory as follows. Macroscopic material parameters, namely, energy of facet planes  $\varepsilon$  and intrinsic surface stress  $\tau_{ij}$  are taken to be different for two materials.

To analyze the instability of planar surfaces and to find the equilibrium orientation of facets, detailed information on the orientational dependence of the surface free energy  $\varepsilon(\hat{\mathbf{m}})$  is needed. This problem is beyond our macroscopic theory.

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<sup>1</sup> C. Herring, Phys. Rev. **82**, 87 (1951).

<sup>2</sup> R.J. Phaneuf and E.D. Williams, Phys. Rev. Lett. **58**, 2563 (1987).

<sup>3</sup> R.J. Phaneuf, E.D. Williams, and N.C. Bartelt, Phys. Rev. B **38**, 1984 (1988).

<sup>4</sup> X.-S. Wang, J.L. Goldberg, N.C. Bartelt, T.L. Einstein, and E.D. Williams, Phys. Rev. Lett. **65**, 2430 (1990).

- <sup>5</sup> R.J. Phaneuf, N.C. Bartelt, E.D. Williams, W. Swiech, and E. Bauer, *Phys. Rev. Lett.* **71**, 2284 (1993).
- <sup>6</sup> E.D. Williams, R.J. Phaneuf, Jian Wei, N.C. Bartelt, and T.L. Einstein, *Surf. Sci.* **294**, 219 (1993).
- <sup>7</sup> M. Kasu and N. Kobayashi, *Appl. Phys. Lett.* **62**, 1262 (1993).
- <sup>8</sup> N.N. Ledentsov, G.M. Gurianov, G.E. Tsyrlin, V.N. Petrov, Yu.B. Samsonenko, A.O. Golubok, and S.Ya. Tipisev, *Fiz. Tekh. Poluprovodn.* **28**, 904 (1994) [*Sov. Phys. Semicond.* **28**, 526 (1994)].
- <sup>9</sup> G.M. Watson, D. Gibbs, D.M. Zehner, M. Yoon, and S.G.J. Mochrie, *Phys. Rev. Lett.* **71**, 3166 (1993).
- <sup>10</sup> R. Koch, M. Borbonus, O. Haase, and K.H. Rieder, *Phys. Rev. Lett.* **67**, 3416 (1991).
- <sup>11</sup> J.-K. Zuo, R.J. Warmack, D.M. Zehner, and J.F. Wendelken, *Phys. Rev. B* **47**, 10743 (1993).
- <sup>12</sup> R. Nötzel, N.N. Ledentsov, L. Däweritz, M. Hohenstein, and K. Ploog, *Phys. Rev. Lett.* **67**, 3812 (1991).
- <sup>13</sup> R. Nötzel, N.N. Ledentsov, L. Däweritz, K. Ploog, and M. Hohenstein, *Phys. Rev. B* **45**, 3507 (1992).
- <sup>14</sup> D.J. Eaglesham and M. Cerullo, *Phys. Rev. Lett.* **64**, 1943 (1990).
- <sup>15</sup> Y.-W. Mo, D.E. Savage, B.S. Swartzentruber, and M.G. Lagally, *Phys. Rev. Lett.* **65**, 1020 (1990).
- <sup>16</sup> D. Leonard, M. Krishnamurthy, C.M. Reaves, S.P. Denbaars, and P.M. Petroff, *Appl. Phys. Lett.* **63**, 3203 (1993).
- <sup>17</sup> N.N. Ledentsov, M. Grundmann, N. Kirstaedter, J. Christen, R. Heitz, J. Böhrer, F. Heinrichsdorff, D. Bimberg, S.S. Ruvimov, P. Werner, U. Richter, U. Gösele, J. Heidenreich, V.M. Ustinov, A.Yu. Egorov, M.V. Maximov, P.S. Kop'ev, and Zh.I. Alferov, in *Proceedings of the 22nd International Conference on the Physics of Semiconductors, Vancouver, Canada, 1994*, edited by D.J. Lockwood (World Scientific, Singapore, 1995), Vol. 3, p. 1855.
- <sup>18</sup> J.M. Moison, F. Houzay, F. Barthe, L. Leprince, E. André, and O. Vatel, *Appl. Phys. Lett.* **64**, 196 (1994).
- <sup>19</sup> A. Madhukar, O. Xie, P. Chen, and A. Konkar, *Appl. Phys. Lett.* **64**, 2727 (1994).
- <sup>20</sup> M.A. Grinfeld, *Dokl. Akad. Nauk SSSR* **290**, 1358 (1986) [*Sov. Phys. Dokl.* **31**, 831 (1986)].
- <sup>21</sup> S. Luryi and E. Suhir, *Appl. Phys. Lett.* **49**, 140 (1986).
- <sup>22</sup> D. Srolovitz, *Acta Metall.* **37**, 621 (1989).
- <sup>23</sup> D. Vanderbilt and L.K. Wickham, in *Evolution of Thin-Film and Surface Microstructure*, edited by C.V. Thompson, J.Y. Tsao, and D.J. Srolovitz, MRS Symposia Proceedings No. 202 (Material Research Society, Pittsburgh, 1991), p. 555.
- <sup>24</sup> V.A. Shchukin, N.N. Ledentsov, P.S. Kop'ev, and D. Bimberg (unpublished).
- <sup>25</sup> V.A. Shchukin, A.I. Borovkov, N.N. Ledentsov, and D. Bimberg, *Phys. Rev. B* **51**, 10104 (1995).
- <sup>26</sup> M. Kirstaedter, N.N. Ledentsov, M. Grundmann, D. Bimberg, V.M. Ustinov, S.S. Ruvimov, M.V. Maximov, P.S. Kop'ev, Zh.I. Alferov, U. Richter, P. Werner, U. Gösele, and J. Heidenreich, *Electron. Lett.* **30**, 1416 (1994).
- <sup>27</sup> V.I. Marchenko, *Zh. Eksp. Teor. Fiz.* **81**, 1141 (1981) [*Sov. Phys. JETP* **54**, 605 (1981)].
- <sup>28</sup> G. Wulff, *Z. Kristallogr. Mineral.* **34**, 449 (1901).
- <sup>29</sup> C. Rottman and M. Wortis, *Phys. Rep.* **103**, 59 (1984).
- <sup>30</sup> V.I. Marchenko and A.Ya. Parshin, *Zh. Eksp. Teor. Fiz.* **79**, 257 (1980) [*Sov. Phys. JETP* **52**, 129 (1980)].
- <sup>31</sup> D.J. Cheng, R.F. Wallis, and L. Dobrzynski, *Surf. Sci.* **43**, 400 (1974).
- <sup>32</sup> M. Lannoo and P. Friedel, in *Atomic and Electronic Structure of Surfaces*, edited by G. Ertl and R. Gomer, Springer Series in Surface Sciences Vol. 16 (Springer-Verlag, Berlin, 1991).
- <sup>33</sup> Zh.I. Alferov, A.Yu. Egorov, A.E. Zhukov, S.V. Ivanov, P.S. Kop'ev, N.N. Ledentsov, B.Ya. Mel'tser, and V.M. Ustinov, *Fiz. Tekh. Poluprovodn.* **26**, 1715 (1992) [*Sov. Phys. Semicond.* **26**, 959 (1992)].
- <sup>34</sup> W. Burton, N. Cabrera, and F. Frank, *Philos. Trans. A* **243**, 299 (1951).
- <sup>35</sup> B. Joós, T.L. Einstein, and N.C. Bartelt, *Phys. Rev. B* **43**, 8153 (1991).
- <sup>36</sup> K. Kern, H. Niehus, A. Schatz, P. Zeppenfeld, J. Goerge, and G. Comsa, *Phys. Rev. Lett.* **67**, 855 (1991).
- <sup>37</sup> V. Bressler-Hill, A. Lorke, S. Varma, P.M. Petroff, K. Pond, and W.H. Weinberg, *Phys. Rev. B* **50**, 8479 (1994).
- <sup>38</sup> V.I. Marchenko, *Pis'ma Zh. Eksp. Teor. Fiz.* **33**, 397 (1981) [*JETP Lett.* **33**, 381 (1981)].
- <sup>39</sup> O.L. Alerhand, D. Vanderbilt, R.D. Meade, and J.D. Joannopoulos, *Phys. Rev. Lett.* **61**, 1973 (1988).
- <sup>40</sup> V.I. Marchenko, *Pis'ma Zh. Eksp. Teor. Fiz.* **55**, 72 (1992) [*JETP Lett.* **55**, 73 (1992)].
- <sup>41</sup> D. Vanderbilt, *Surf. Sci.* **268**, L300 (1992).
- <sup>42</sup> P. Zeppenfeld, M. Krzyzowski, C. Romainczyk, G. Comsa, and M.G. Lagally, *Phys. Rev. Lett.* **72**, 2737 (1994).
- <sup>43</sup> L.D. Landau and E.M. Lifshitz, *Theory of Elasticity* (Pergamon, New York, 1980).
- <sup>44</sup> M. Wassermeier, J. Sudijono, M.D. Johnson, K.T. Leung, B.G. Orr, L. Däweritz, and K. Ploog (unpublished).
- <sup>45</sup> O. Brandt, K. Ploog, R. Bierwolf, and M. Hohenstein, *Phys. Rev. Lett.* **68**, 1339 (1992).
- <sup>46</sup> A.A. Baski and L.J. Whitman, *Phys. Rev. Lett.* **74**, 956 (1995).
- <sup>47</sup> L. De Caro and L. Tapfer, *Phys. Rev. B* **48**, 2298 (1993).
- <sup>48</sup> S.-H. Wei and A. Zunger, *Phys. Rev. Lett.* **61**, 1505 (1988).
- <sup>49</sup> A.I. Borovkov, P.V. Ilyin, Yu. Krivchenkov, A. Panin, and G. Sivkova, *IEEE Trans. Magn.* **28**, 927 (1992).
- <sup>50</sup> M.C. Payne, N. Roberts, R.J. Needs, M. Needels, and J.D. Joannopoulos, *Surf. Sci.* **211**, 1 (1989).
- <sup>51</sup> J. Dabrowski, E. Pehlke, and M. Scheffler, *Phys. Rev. B* **49**, 4790 (1994).
- <sup>52</sup> A. Madhukar (private communication).