Tuning and breakdown of faceting under externally applied stress

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(Received 8 August 1994; revised manuscript received 28 December 1994)

The theory of thermodynamic faceting is developed for an epitaxial film grown coherently on a lattice-mismatched substrate. The situation is considered where the planar top surface of the epitaxial film in the absence of the lattice mismatch ($\Delta a = 0$) is unstable against faceting, and the stable state of the surface is a periodic array of facets. It is shown that, for a finite lattice mismatch ($\Delta a \neq 0$), the continuous epitaxial film with a periodically faceted top surface is a metastable state of the heterophase system. The global energy minimum corresponds then to a periodic system of coherent strained islands. If attaining the global energy minimum is kinetically forbidden, the metastable continuous epitaxial film with a periodically faceted top surface is formed. In the case where the period of the faceted structure *without external stress* L_0 exceeds the order of $\approx$50 Å, the dependence of the period L on the lattice mismatch is determined by the linear theory of elasticity. The period L of the metastable faceted structure increases with $|\Delta a|$ for both tensile and compressive mismatch-induced strain. The dependence of L on Δa gives a possibility of controlling the period of faceting by varying Δa. If the lattice mismatch exceeds a certain critical value [$|\Delta a| > (\Delta a)_c$], the breakdown of formation of metastable faceted structures occurs; the metastable state disappears, and the surface shape is governed by kinetic mechanism. In the case where the period of the faceted structure *without external stress* is $L_0 \lesssim 50$ Å, the dependence of L on Δa is determined by nonlinear elastic effects. The period L increases for one sign of Δa up to the breakdown of formation of metastable faceted structures and decreases for the other sign of Δa, where the macroscopic faceting transforms gradually into a microscopic surface reconstruction and the surface becomes apparently flat. The typical critical value of the lattice mismatch for nanometer-scale faceting varies from $(\Delta a/a)_c \sim 10^{-4}$ for $L \sim 10^3$ Å to $(\Delta a/a)_c \sim 10^{-2}$ for $L \sim 10$ Å. A similar dependence of faceting on externally applied stress occurs for a loaded sample.

I. INTRODUCTION

Equilibrium faceting is a remarkable phenomenon, in which a planar crystal surface rearranges into a periodic hill-and-valley structure with an increased surface area. Faceting is caused by the decrease of the total surface free energy.[1] 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) (Refs. 2–6) (the detailed review is given by Williams *et al.*[7]). Faceting was observed also on vicinals to GaAs(100) (Refs. 8 and 9), Pt(100),[10] on low-index singular surfaces Ir(110),[11] TaC(110),[12] on non-(100)-oriented GaAs,[13,14] 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 the Ge/Si(001) system,[15,16] in the $In_{1-x}Ga_xAs$/GaAs(001) system,[17,18] and in the InAs/GaAs(001) system.[18–20] The growth of coherent strained islands was explained theoretically by the instability of planar surfaces in stressed systems.[21–25] 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[24] and may lead to an ordered array of coherent islands.[26] Recent interest in surface faceting and other related phenomena is stimulated by possibilities of the direct fabrication of ordered arrays of quantum wires and quantum dots with novel physical properties and device applications.[27]

0163-1829/95/51(15)/10104(15)/$06.00

The objective of the present paper is to consider the *effect* of externally applied stress on the type of faceting where faceting of the surface initially occurs *without* any external stress. The treatment is focused on thermodynamic mechanism of faceting where the shape of the surface is governed by the Helmholtz free energy minimum.

The Helmholtz free energy of a faceted surface *without external stress* was studied by Marchenko.[28] It was shown that the surface free energy consists of three terms,

$$F = E_{\text{facets}} + E_{\text{edges}} + E_{\text{elastic}}\,, \tag{1}$$

E_{facets} being the free energy of facets, E_{edges} being the short-range energy of crystal edges, and E_{elastic} being the elastic strain energy associated with 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. 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_{facets}, is proportional to the surface area. The energy of edges E_{edges} is less than E_{facets} due to the small parameter $a/L_F \ll 1$. In the absence of the lattice mismatch ($\Delta a = 0$), the elastic strain energy is caused by edges only, and is small with respect to E_{facets}, due to the same small parameter $a/L_F \ll 1$.

The energy E_{facets} was studied in detail by Herring and others.[1,29,30] The equilibrium crystal shape is determined by the Wulff construction,[29] which implies the minimization 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 experimental situation where only the top surface of a crystal is studied, or to the epitaxial growth. 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:[1,30]

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

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,

$$\frac{1}{S}\int \hat{\mathbf{m}}dS = \hat{\mathbf{n}}\,. \tag{3}$$

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 the elastic strain energy. We focus here on the case of sharp edges. Macroscopic treatment is possible also for rounded intersections between facets.

Let us specify energies E_{edges} and E_{elastic} for the particular case of faceted structures which 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, φ being the tilt angle of facets. Small energy terms $E_{\text{edges}} + E_{\text{elastic}}$ do not affect the tilt angle φ. However, it was shown by Marchenko[28] that the minimum of the free energy (1), where both E_{edges} and E_{elastic} are taken into account, corresponds to the periodic array of facets. The energies E_{edges} and E_{elastic} depend on the period L, and the interplay of these energies determines the optimum period of surface corrugation. Thus, a periodic array of facets is an example of a structure of stress domains.

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,

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

Elastic strain energy in the system with corrugated surface occurs due to the intrinsic surface stress (or the surface tension of the solid). The strain energy of the system defined per unit area of the reference flat surface is then equal to[31]

$$E_{\text{elastic}} = \frac{1}{2S}\int \lambda_{ijlm}\varepsilon_{ij}(\mathbf{r})\varepsilon_{lm}(\mathbf{r})dV + \frac{1}{S}\int \tau_{ij}(\mathbf{r})\varepsilon_{ij}(\mathbf{r})dS\,. \tag{5}$$

Here, $\varepsilon_{ij}(\mathbf{r})$ is the strain tensor, λ_{ijlm} is the tensor of elastic moduli, $\tau_{ij}(\mathbf{r})$ is the intrinsic surface stress tensor. The intrinsic surface-stress tensor τ_{ij} depends on the orientation of the facet (see Fig. 2). It has nonzero components τ_{ij} in the facet plane, and the other components vanish. The tensor τ_{ij} is constant on the given facet and has discontinuities at crystal edges separating neighboring facets. The discontinuity of the tensor τ_{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:[28] $E_{\text{elastic}} = -(2S)^{-1}\int \mathbf{u}_i(\mathbf{r})\nabla_\beta\tau_{i\beta}(\mathbf{r})dS$, $\mathbf{u}_i(\mathbf{r})$ being the displacement vector, β being the planar index in the local facet plane. The sources of the strain field may be described as effective elastic forces $\mathbf{P}$ applied to

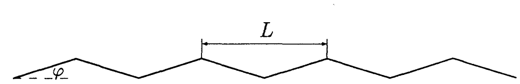

FIG. 1. One-dimensional array of facets.

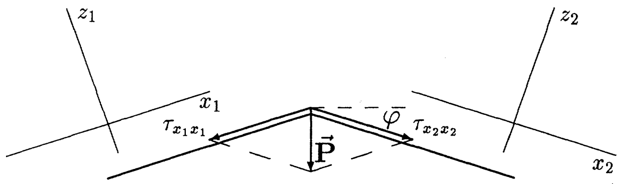

FIG. 2. Effective "surface-stress" forces at crystal edges. The tensor τ_{ij} is defined in local systems of coordinates (x_1, y, z_1) and (x_2, y, z_2). For a symmetric sawtooth profile, $\tau_{x_1x_1} = \tau_{x_2x_2} = \tau$; $P_x = 0$, $P_z = -2\tau \sin\varphi$.

crystal edges. The relation between $\mathbf{P}$ and τ_{ij}, illustrated in Fig. 2, reads $P = 2\tau \sin\varphi$.

It should be noted that strain field occurs also in the case of a planar surface. Elastic relaxation near planar surface results in static displacements of atoms from their bulk positions. These displacements decay exponentially at the depth of a few lattice constants.[32] The same is valid also for static displacements of atoms caused by microscopic surface reconstruction (see, e.g., Ref. 33). 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 $\mathbf{P}$ caused by the discontinuity of the intrinsic surface-stress tensor τ_{ij} 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_{elastic} in the case of small tilt angle φ of facets was calculated in Ref. 28 by means of the continuum theory of elasticity in the approximation of elastically isotropic medium. The strain energy is given in terms of the intrinsic surface stress τ, the Young's modulus Y and the Poisson ratio ν as follows:

$$E_{\mathrm{elastic}}(L) = - \frac{8(1-\nu^2)\tau^2\varphi^2}{\pi Y L} \ln\left(\frac{L}{2\pi a}\right) , \qquad (6)$$

a being a microscopic cutoff length which is of the order of the lattice constant. The physical meaning of the strain energy (6) is the energy change due to elastic relaxation, the relaxation being caused by the discontinuity of the tensor τ_{ij} at crystal edges. Since the relaxation occurs spontaneously, the sign of the strain energy is negative. The logarithmic dependence of the elastic strain energy (6) on L is a general feature of any linear defect. It remains in the case of rounded edges, too. For large tilt angles φ, the energy E_{elastic} may be calculated numerically.

Summing contributions of Eqs. (2,4,6), we may write down the total surface free energy as follows:

$$E = \frac{\varepsilon(\varphi)}{\cos\varphi} + \frac{C_1(\varphi)}{L} - \frac{C_2(\varphi)}{L} \ln\left(\frac{L}{2\pi a}\right) . \qquad (7)$$

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 which depends on the angle φ, $g(0;\nu) = 1$. The energy (7) attains the minimum value at

$$L_0 = 2\pi a \, \exp\left[\frac{C_1(\varphi)}{C_2(\varphi)} + 1\right] . \qquad (8)$$

It will be shown below that the ratio of two functions $C_1(\varphi)/C_2(\varphi)$ tends to a finite limit as $\varphi \to 0$.

Since the optimum period of surface corrugation L_0 is determined by long-range stresses, it should vary if external stress is applied. The dependence of the period L on applied external stress was observed experimentally by Men *et al.*[34] and explained theoretically by Alerhand *et al.*[35] for another type of elastic stress domain, namely, for alternating domains of the (2×1)- and the (1×2)-reconstructed Si(100) surface.

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 the temperature $T = 0$. Entropy effects in the free energy of a faceted surface, which appear at finite temperatures, were considered in Ref. 36. It was shown that entropy effects for macroscopically faceted surface are less essential than for a vicinal stepped surface and, hence, can be neglected. Then the free energy of the surface is equal to the energy of the surface.

We study in the present paper thermodynamic faceting of surfaces under an externally applied stress. For above noted reasons, we do not take into account the entropy contribution into the Helmholtz free energy of the faceted surface and we search the minimum of the energy of the faceted surface under external stress. Two different ways of applying stress are considered. An epitaxial film coherently grown on a lattice-mismatched substrate is treated in Sec. II. There are then two sources of the strain field, i.e., effective forces $\mathbf{P}$ acting at crystal edges, and the lattice mismatch $\Delta a/a$. The elastic strain energy E_{elastic} is a quadratic function of $\mathbf{P}$ and $\Delta a/a$. It is shown that the surface energy minimum at $L = L_0$, which is the absolute minimum in the absence of the lattice mismatch $(\Delta a = 0)$, becomes a local minimum for a finite Δa and is shifted to larger values of L. The global minimum corresponds then to a periodic array of isolated coherent strained islands. The continuous epitaxial film with the periodically corrugated top surface is then a metastable state of the heterophase lattice-mismatched system. This metastable state may be called a "metastable faceted structure."

It should be noted that, to use an unambiguous terminology, we distinguish here the "metastable faceting" and the "formation of a metastable faceted structure." Terms "metastable faceting" and "unstable faceting" (see, e.g., Ref. 6) refer to the first energy term in Eq. (1), i.e., to the energy of planar facets. "Metastable faceting" means that there exists a potential barrier which separates the flat surface and the faceted surface with lower free energy, and the transformation of the flat surface into the faceted one occurs via nucleation-and-growth mechanism. "Unstable faceting" means that there is no potential barrier between the flat surface and the faceted surface. Then the transformation of the flat surface into the faceted one is analogous to spinodal decomposition observed in other phase separating systems, e.g., in unstable alloys.[37] In both cases, the faceted surface itself is a stable one if the short-range energy of edges and the strain energy are ignored.

Contrary to this, we study here faceted structures with given orientation of facets [first energy term in Eq. (1) being fixed], and we do not focus on the particular scenario of transformation of the flat surface into the faceted one. "Formation of a metastable faceted structure" means that the heterophase structure with a periodic array of facets is metastable with respect to rearrangement of facet widths. This rearrangement influences the energy of edges and the strain energy, i.e., the second and the third energy terms in Eq. (1).

We have found that, if the lattice mismatch exceeds a certain critical value, $[|\Delta a| > (\Delta a)_c]$, the local minimum in the total surface energy disappears, which indicates the breakdown of formation of metastable faceted structures.

In Sec. III, the elastic strain energy and the critical value of the lattice mismatch are found in an analytic form for a faceted structure with a small tilt angle of facets φ. The numerical analysis is performed for an arbitrary angle φ for the particular AlAs(001) faceted surface.

Due to the strong dependence of intrinsic parameters of the crystal (e.g., the energy of crystal edges) on strain, the faceting under externally applied stress is determined by nonlinear elastic effects, if the period of faceting without external stress is rather small, $L_0 \lesssim 50$ Å. The period of the metastable faceted structure L found in Sec. IV exhibits then an asymmetric dependence on Δa. For one sign of the lattice mismatch, the period L increases with $|\Delta a|$ up to the breakdown of formation of metastable faceted structures. For another sign of the lattice mismatch, the period L decreases with $|\Delta a|$. The depth of surface corrugation decreases then, too, unless the macroscopically faceted surface transforms into the microscopically reconstructed, i.e., apparently flat surface.

An alternative way of applying stress to the system is loading the sample (particularly, the loading of a cantilevered bar of Si was studied experimentally in Ref. 34). The dependence of faceting on external load is studied in Sec. V and is shown to be similar to that in the case of a mismatched heterostructure.

II. FACETING OF THE SURFACE OF AN EPITAXIAL FILM ON A LATTICE-MISMATCHED SUBSTRATE

We study first the elastic strain energy of a faceted surface of a thin epitaxial film grown coherently on a lattice-mismatched substrate (Fig. 3). There are two sources of the strain field in this case. One is due to effective external forces acting at crystal edges, these forces arising from the discontinuity of intrinsic surface stress tensor at edges. The other source is due to the lattice mismatch. To treat the lattice mismatch it is convenient

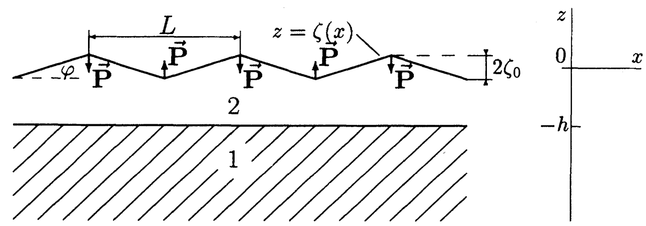

FIG. 3. Faceted surface of the epitaxial film (2) coherently grown on a lattice-mismatched substrate (1).

to use the quantity of the intrinsic strain $\varepsilon_{ij}^{(0)}(\mathbf{r})$ defined by the difference of intrinsic lattice parameters of two materials.[38–41] The intrinsic strain $\varepsilon_{ij}^{(0)}(\mathbf{r})$ vanishes in the substrate (region 1 in Fig. 3) and differs from zero in the epitaxial film (region 2 in Fig. 3). Note that $\varepsilon_{ij}^{(0)}(\mathbf{r}) = 0$ does not mean the rigid substrate. Although all sources of the strain field appear either in the epitaxial film, or at the interface, or on the corrugated top surface, the strain field penetrates into the substrate, too. The elastic energy density $f_{\text{elastic}}(\mathbf{r})$ at each point in the bulk is caused by the deviation of the local strain $\varepsilon_{ij}(\mathbf{r})$ from the local intrinsic strain $\varepsilon_{ij}^{(0)}(\mathbf{r})$,

$$f_{\text{elastic}}(\mathbf{r}) = \frac{1}{2}\lambda_{ijlm}[\varepsilon_{ij}(\mathbf{r}) - \varepsilon_{ij}^{(0)}(\mathbf{r})][\varepsilon_{lm}(\mathbf{r}) - \varepsilon_{lm}^{(0)}(\mathbf{r})] \,. \tag{9}$$

It is assumed for simplicity that elastic moduli λ_{ijlm} in the epitaxial film and in the substrate coincide. The elastic stress is equal by definition to

$$\sigma_{ij}(\mathbf{r}) = \frac{\partial f_{\text{elastic}}}{\partial \varepsilon_{ij}(\mathbf{r})} = \lambda_{ijlm}[\varepsilon_{lm}(\mathbf{r}) - \varepsilon_{lm}^{(0)}(\mathbf{r})] \,. \tag{10}$$

It follows from Eq. (10) that the stress-free state $[\sigma_{ij}(\mathbf{r}) = 0]$ inside the epitaxial film corresponds to the strained state of the medium, $\varepsilon_{ij}(\mathbf{r}) = \varepsilon_{ij}^{(0)}(\mathbf{r}) \neq 0$.

The contribution of intrinsic surface stress into the elastic strain energy of the system occurs if the local strain $\varepsilon_{ij}(\mathbf{r})$ near the surface deviates from the local intrinsic strain $\varepsilon_{ij}^{(0)}(\mathbf{r})$. To write down this contribution one should take the energy of the second term on the right hand side of Eq. (5) and substitute $\varepsilon_{ij}(\mathbf{r})$ by $[\varepsilon_{ij}(\mathbf{r}) - \varepsilon_{ij}^{(0)}(\mathbf{r})]$. One gets

$$\frac{1}{S}\int \tau_{ij}(\mathbf{r})[\varepsilon_{ij}(\mathbf{r}) - \varepsilon_{ij}^{(0)}(\mathbf{r})]dS \,. \tag{11}$$

To obtain the total elastic strain energy of the heterophase system E_{elastic} one should integrate the elastic energy density from Eq. (9) over the total volume of the system and add the energy from Eq. (11):

$$E_{\text{elastic}} = \frac{1}{2S}\int\int dxdy \int_{-\infty}^{\zeta(x)} dz \lambda_{ijlm}[\varepsilon_{ij}(\mathbf{r}) -\varepsilon_{ij}^{(0)}(\mathbf{r})][\varepsilon_{lm}(\mathbf{r}) - \varepsilon_{lm}^{(0)}(\mathbf{r})] + \frac{1}{S}\int_{z=\zeta(x)} dS\tau_{ij}(\mathbf{r})[\varepsilon_{ij}(\mathbf{r}) - \varepsilon_{ij}^{(0)}(\mathbf{r})]\,. \quad (12)$$

In the absence of the lattice mismatch [in the case where $\varepsilon_{ij}^{(0)}(\mathbf{r}) = 0$], the elastic energy E_{elastic} from Eq. (12) gives just the contribution of edges into the strain energy [the third term in Eq. (7)]. Mismatch-induced strains give the positive contribution to E_{elastic}.

Since elastic stresses penetrate from the epitaxial film into the substrate, the domain of integration in the first term on the right hand side of Eq. (12) $[-\infty < z < \zeta(x)]$ (see Fig. 3) includes both the film $[-h < z < \zeta(x)]$ and the substrate $(-\infty < z < -h)$ although the intrinsic strain $\varepsilon_{ij}^{(0)}(\mathbf{r})$ in the substrate vanishes. Given the spatial distribution of the effective external forces $P_i(\mathbf{r})$ and of the intrinsic strain $\varepsilon_{ij}^{(0)}(\mathbf{r})$, the strain field $\varepsilon_{ij}(\mathbf{r}) = \frac{1}{2}[\nabla_j u_i(\mathbf{r}) + \nabla_i u_j(\mathbf{r})]$ is determined by the minimization of E_{elastic} (12) with respect to independent variables $u_i(\mathbf{r})$, $u_i(\mathbf{r})$ being the displacement vector. The requirement of total elastic energy minimum yields equilibrium equations of the theory of elasticity, $\nabla_j \sigma_{ij}(\mathbf{r}) = 0$, which correspond to the absence of external forces in the bulk. Substituting here $\sigma_{ij}(\mathbf{r})$ from Eq. (10) yields the set of coupled equations with respect to the displacement vector $u_i(\mathbf{r})$:

$$\frac{\partial}{\partial r_j}\left(\lambda_{ijlm}\frac{\partial}{\partial r_l}u_m(\mathbf{r})\right) = \frac{\partial}{\partial r_j}(\lambda_{ijlm}\varepsilon_{lm}^{(0)}(\mathbf{r}))\,. \quad (13)$$

The boundary conditions

$$\lambda_{ijlm}n_j(\mathbf{r})\frac{\partial}{\partial r_l}u_m(\mathbf{r})\bigg|_{z=\zeta(x)} = \lambda_{ijlm}n_j(\mathbf{r})\varepsilon_{lm}^{(0)}(\mathbf{r})|_{z=\zeta(x)} - P_i(\mathbf{r})|_{z=\zeta(x)}\,, \quad (14)$$

$[n_j(\mathbf{r})$ being the normal vector to the free surface$]$ connect the stress at the free surface $z = \zeta(x)$ and effective external forces acting at edges $P_i(\mathbf{r}) = -\nabla_\beta \tau_{i\beta}(\mathbf{r})$.

To proceed, we transform Eq. (12) by the method suggested by Eshelby.[42] Applying the Gauss theorem both to the bulk and the surface integrals in Eq. (12), using the equilibrium equations (13) and boundary conditions (14), one obtains the elastic energy as follows:

$$E_{\text{elastic}} = \frac{1}{2S}\int\int dxdy\int_{-h}^{\zeta(x)} dz\lambda_{ijlm}\varepsilon_{ij}^{(0)}(\mathbf{r})[\varepsilon_{lm}^{(0)}(\mathbf{r}) - \varepsilon_{lm}(\mathbf{r})] - \frac{1}{2S}\int_{z=\zeta(x)} dSP_i(\mathbf{r})u_i(\mathbf{r}) - \frac{1}{S}\int_{z=\zeta(x)} dS\tau_{ij}(\mathbf{r})\varepsilon_{ij}^{(0)}(\mathbf{r})\,. \quad (15)$$

Here, the domain of integration corresponds, at the contrary to Eq. (12), only to the epitaxial film where the intrinsic strain $\varepsilon_{ij}^{(0)}(\mathbf{r})$ does not vanish. Since the intrinsic strain $\varepsilon_{ij}^{(0)}(\mathbf{r})$ is uniform inside the epitaxial film, Eq. (15) reduces to

$$E_{\text{elastic}} = \frac{1}{2}\lambda_{ijlm}\varepsilon_{ij}^{(0)}\varepsilon_{lm}^{(0)}h - \frac{1}{2L_x}\lambda_{ijlm}\varepsilon_{lm}^{(0)}\int dx\int_{-h}^{\zeta(x)} dz\varepsilon_{ij}(x,z) - \frac{1}{2L_x}\int dlP_i(x)u_i(x,\zeta(x)) - \frac{1}{L_x}\varepsilon_{ij}^{(0)}\int dl\tau_{ij}(x)\,, \quad (16)$$

where $dl \equiv \sqrt{1 + (\nabla\zeta(x))^2}dx$ is the elementary length of the cross section of the corrugated surface $z = \zeta(x)$ by the (xz) plane; L_x is the length of the sample.

The first term on the right hand side of Eq. (16) is a film-thickness contribution to E_{elastic}, which increases with the thickness h. The second term contains both film-thickness and surface contributions, the latter does not increase with h. The third and the fourth terms are purely surface contributions. To separate film-thickness and surface contributions into E_{elastic}, we consider first the strain field in the epitaxial film with a flat top surface.

The strain field in the epitaxial film with a flat top surface coherently grown on a lattice-mismatched substrate was treated in numerous papers (see, e.g., Ref. 43 and references therein). The strain in the film is uniform and obeys the following equations:

$$\widetilde{\varepsilon_{ab}} = 0\,, \quad a,b = x,y\,, \quad (17)$$

$$\widetilde{\sigma_{iz}} = \lambda_{izlm}(\widetilde{\varepsilon_{lm}} - \varepsilon_{lm}^{(0)}) = \lambda_{izlz}\widetilde{\varepsilon_{lz}} - \lambda_{izlm}\varepsilon_{lm}^{(0)} = 0\,. \quad (18)$$

The set of three coupled equations (18) determines the values of three nonvanishing components $\widetilde{\varepsilon_{lz}}$ of the strain tensor. The displacement vector in the system is then equal to

$$\widetilde{u_a}(\mathbf{r}) = 2\widetilde{\varepsilon_{az}}(z+h)\vartheta(z+h),$$

$$\widetilde{u_z}(\mathbf{r}) = \widetilde{\varepsilon_{zz}}(z+h)\vartheta(z+h)\,, \quad (19)$$

[where $\vartheta(x) = 1$ for $x > 0$, and $\vartheta(x) = 0$ for $x < 0$], and the stress tensor $\widetilde{\sigma_{ij}}$ has nonvanishing in-plane components,

$$\widetilde{\sigma_{ab}} = \lambda_{ablm}\left(\widetilde{\varepsilon_{lm}} - \varepsilon_{lm}^{(0)}\right) = \lambda_{ablz}\widetilde{\varepsilon_{lz}} - \lambda_{ablm}\varepsilon_{lm}^{(0)}\,. \quad (20)$$

Now, to solve the problem for an epitaxial film with corrugated surface, we write down the displacement vector $u_i(\mathbf{r})$ as a sum of $\widetilde{u_i}(\mathbf{r})$ from Eq. (19) and of an unknown vector $w_i(\mathbf{r})$, $u_i(\mathbf{r}) = \widetilde{u_i}(\mathbf{r}) + w_i(\mathbf{r})$, and then substitute it into Eqs. (13,14). Then one gets the following set of coupled equations for the vector $w_i(\mathbf{r})$:

$$\lambda_{ijlm}\frac{\partial^2}{\partial r_j \partial r_l}w_m(\mathbf{r}) = 0\,, \quad (21)$$

with the boundary conditions at the free surface,

$$\lambda_{ijlm} n_j(\mathbf{r}) \frac{\partial}{\partial r_l} w_m(\mathbf{r}) \bigg|_{z=\zeta(x)} = -\widetilde{\sigma_{ix}} n_x(\mathbf{r}) + P_i(\mathbf{r}) \,, \quad (22)$$

[the quantity $\widetilde{\sigma_{ix}}$ is defined in Eqs. (18,20)]. The solution of Eq. (21) may be expressed in terms of the Green's tensor $G_{ij}(\mathbf{r}, \mathbf{r}')$ of the semi-infinite medium with the faceted surface $z = \zeta(x)$. The Green's tensor obeys the set of coupled equations,

$$\lambda_{ijlm} \frac{\partial}{\partial r_j} \frac{\partial}{\partial r_l} G_{mp}(\mathbf{r}, \mathbf{r}') = \delta_{ip} \delta(\mathbf{r} - \mathbf{r}') \,, \quad (23)$$

and boundary conditions

$$\lambda_{ijlm} n_j(\mathbf{r}) \frac{\partial}{\partial r_l} G_{mp}(\mathbf{r}, \mathbf{r}') \bigg|_{z=\zeta(x)} = 0 \,. \quad (24)$$

Substituting the vector

$$w_i\Big(x, z\Big) = - \int dl' G_{ij}(x, z; x', \zeta(x')) \times [P_j(x') - \widetilde{\sigma_{jx}} n_x(x')] \quad (25)$$

into Eq. (16), applying the Gauss theorem to the integral over the volume of the epitaxial film, taking into account the total balance of the surface-stress forces, $\int dS P_i(\mathbf{r}) = 0$, and the constraint (3) which reads $\int dS n_x(\mathbf{r}) = 0$, one gets the elastic energy of the system in the following form:

$$E_{\text{elastic}} = E^{\text{film}}_{\text{elastic}} + E^{\text{surf}}_{\text{elastic}} \,. \quad (26)$$

Here, $E^{\text{film}}_{\text{elastic}} = \frac{1}{2} \lambda_{ijlm} \varepsilon^{(0)}_{ij} (\varepsilon^{(0)}_{lm} - \widetilde{\varepsilon_{lm}}) Sh$ is the film-thickness contribution to E_{elastic}, which does not depend on the shape of the free surface. The remaining part of E_{elastic} is equal to

$$\begin{aligned}
E^{\text{surf}}_{\text{elastic}} = & - \frac{1}{L_x} \varepsilon^{(0)}_{ij} \int dl \tau_{ij}(x) && \text{(27a)} \\
& - \frac{1}{L_x} \widetilde{\varepsilon_{xz}} \int dx P_x(x) \zeta(x) - \frac{1}{L_x} \frac{\widetilde{\varepsilon_{zz}}}{2} \int dx P_z(x) \zeta(x) && \text{(27b)} \\
& + \frac{1}{2L_x} \int \int dl dl' P_i(x) G_{ij}(x, \zeta(x); x', \zeta(x')) P_j(x') && \text{(27c)} \\
& - \frac{1}{2L_x} \int \int dl dl' P_i(x) G_{ij}(x, \zeta(x); x', \zeta(x')) \widetilde{\sigma_{jx}} n_x(x') && \text{(27d)} \\
& + \frac{1}{2L_x} \int \int dl dl' \sigma^{(0)}_{il} n_l(x) G_{ij}(x, \zeta(x); x', \zeta(x')) P_j(x') && \text{(27e)} \\
& - \frac{1}{2L_x} \int \int dl dl' \sigma^{(0)}_{il} n_l(x) G_{ij}(x, \zeta(x); x', \zeta(x')) \widetilde{\sigma_{jx}} n_x(x') && \text{(27f)} \\
& - \frac{1}{2L_x} \int \int dx dl' \sigma^{(0)}_{iz} G_{ij}(x, -h; x', \zeta(x')) [P_j(x') - \widetilde{\sigma_{jx}} n_x(x')] \,, && \text{(27g)}
\end{aligned}$$

where $\sigma^{(0)}_{ij}$ is defined as $\sigma^{(0)}_{ij} \equiv \lambda_{ijlm} \varepsilon^{(0)}_{lm}$.

It follows from Eqs. (21,22) that all sources of the vector $w_i(\mathbf{r})$ are surface sources, and the vector $w_i(\mathbf{r})$ decays with the depth from the surface. The vector $w_i(\mathbf{r})$ which is a periodic function of x may be expressed at $z < -\zeta(x)$ as a Fourier series,

$$w_i(x, z) = \sum_{\substack{n=-\infty \\ n \neq 0}}^{+\infty} \sum_{s=1}^{3} b_s(n) \exp\Big(- \alpha_s |n| k^{(0)}_x |z| \Big) \times \exp\Big(i n k^{(0)}_x x \Big) \,, \quad (28)$$

where $k^{(0)}_x = 2\pi \big/ L$, and α_s $(s = 1, 2, 3)$ are dimensionless attenuation coefficients of static analogs of Rayleigh waves (see, e.g., Ref. 44). The term of Eq. (27g), which depends on the film thickness can be written as follows: $\frac{1}{2} L_y \sigma^{(0)}_{iz} \int dx w_i(x; -h)$. Since the Fourier series of Eq. (28) does not contain x-independent term with $n = 0$, the integral $\int dx w_i(x; -h)$ vanishes. Therefore, the remaining terms of Eq. (27) which do not depend on the epitaxial film thickness h, are, indeed, surface contributions to E_{elastic}.

Let us recall now that the effective elastic forces $\mathbf{P}$ acting at crystal edges are related to components of the intrinsic stress tensor τ_{ij} (see Fig. 2). Therefore, the energy $E^{\text{surf}}_{\text{elastic}}$ from Eq. (27) may be considered either as a quadratic function of P_i and $\varepsilon^{(0)}_{ij}$, or as a quadratic function of τ_{ij} and $\varepsilon^{(0)}_{ij}$. To analyze the general dependence of $E^{\text{surf}}_{\text{elastic}}$ on the lattice mismatch, we consider the particular case where both the substrate and the epitaxial film have cubic symmetry, and the intrinsic strain tensor $\varepsilon^{(0)}_{ij}$ reduces to $\varepsilon^{(0)}_{ij} = (\Delta a / a) \delta_{ij}$. It is then possible to write $E^{\text{surf}}_{\text{elastic}}$ in a schematic form:

$$E^{\text{surf}}_{\text{elastic}} = A(L) \tau^2 + B(L) \tau \left(\frac{\Delta a}{a} \right) + C(L) \left(\frac{\Delta a}{a} \right)^2 \,. \quad (29)$$

Simple scaling arguments performed in Appendix A yield the dependence of coefficients A, B, C in Eq. (29) on the period of the faceted structure L. Then the elastic strain energy defined per unit area of the substrate is as follows:

$$E_{\text{elastic}}^{\text{surf}} = -A\frac{1}{L}\ln\left(\frac{L}{2\pi a}\right)\tau^2 - B\tau\left(\frac{\Delta a}{a}\right) - CL\left(\frac{\Delta a}{a}\right)^2 . \tag{30}$$

The first term on the right hand side of Eq. (30) coincides with the third term of Eq. (7). It is the energy change due to elastic relaxation caused by the discontinuity of the intrinsic surface-stress tensor τ_{ij} at edges. This term is always negative.

The third term on the right hand side of Eq. (30) is the change of the strain energy $E_{\text{elastic}}^{\text{film}}$ due to the surface corrugation. Since the corrugation of the surface of the stressed film always leads to the reduction of the strain energy,[23,24] the third term in Eq. (30) is always negative. The second term in Eq. (30) is a cross term, and it may be of arbitrary sign.

To obtain the total surface energy of the system in question, one should replace the last term on the right hand side of Eq. (1) by $E_{\text{elastic}}^{\text{surf}}$ from Eq. (30). Then the L-dependent part of the energy may be written as a universal function of the dimensionless variable $\left(L/L_0\right)$, the function being governed by a control parameter $(\Delta a/a)\big/(\Delta a/a)_c$:

$$E(L) = E_0\left[-\frac{L_0}{L}\ln\frac{eL}{L_0} - \frac{1}{2e}\left[\frac{(\Delta a/a)}{(\Delta a/a)_c}\right]^2\frac{L}{L_0}\right] . \tag{31}$$

The function $E(L)$ is plotted in Fig. 4 for various values of the lattice mismatch. The absolute minimum of the function at $L = L_0$ for the lattice-matched substrate ($\Delta a = 0$) becomes the local minimum for a finite mismatch and is shifted to larger values of the period. At large periods L, the energy $E(L)$ from Eq. (31) decreases with L. If the amount of the deposited material and the tilt angle of facets are fixed, there exists the maximum possible period L, where the epitaxial film is still continuous. It is determined by the relation

$$\frac{1}{2}L_{\max}\tan\varphi = h . \tag{32}$$

Larger periods $L > L_{\max}$ correspond to periodic arrays of isolated strained islands, and not to a continuous film. Since the absolute value of the third term in Eq. (31) is proportional to the period L, it may compete with the surface energy of facets and may influence the tilt angle of facets. The case of large values of L and the global minimum of the energy of the lattice-mismatched heterophase system will be considered elsewhere.

In reality, attaining of the global minimum of the energy would involve mass transfer on large distances and may be kinetically forbidden. Then the metastable faceted structure may be formed. The period L corresponds then to the local minimum of $E(L)$. The plot $L = L((\Delta a/a))$ is presented in Fig. 5. Since the linear in $\Delta a/a$ term in Eq. (30) does not depend on L, then the period of the metastable faceted structure is an even function of the lattice mismatch. If the lattice mismatch is larger than the critical value $(\Delta a/a)_c$, the metastable state disappears, and the surface shape is governed by kinetic factors. This indicates the breakdown of formation of metastable faceted structures.

The explicit calculation of the critical value of the lattice mismatch will be carried out below, in Sec. III, for a faceted surface with small tilt angle of facets.

In the case where elastic moduli of the epitaxial film are different from those of the substrate, additional terms of the order of $\exp\left[-2(\text{Re}\alpha_s)\frac{2\pi h}{L}\right]$ appear in the Green's tensor $G_{ij}(x,\zeta(x);x',\zeta(x'))$, and, therefore, in $E_{\text{elastic}}^{\text{surf}}$. Then the linear in $\Delta a/a$ term in $E_{\text{elastic}}^{\text{surf}}$ depends on L,

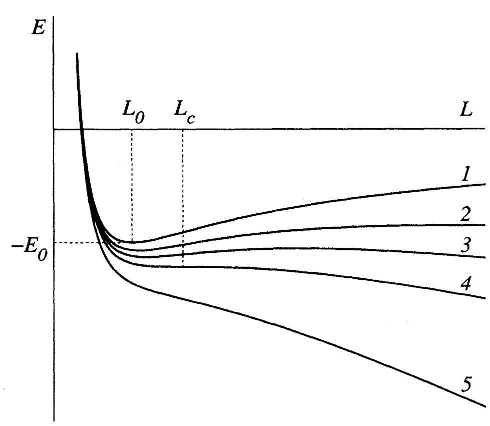

FIG. 4. Surface energy of the faceted surface versus period of faceting for different values of the lattice mismatch (linear theory of elasticity); (1) $\Delta a/a = 0$; (2) $\Delta a/a = 0.6(\Delta a/a)_c$; (3) $\Delta a/a = 0.8(\Delta a/a)_c$; (4) $\Delta a/a = (\Delta a/a)_c$; (5) $\Delta a/a = 1.4(\Delta a/a)_c$.

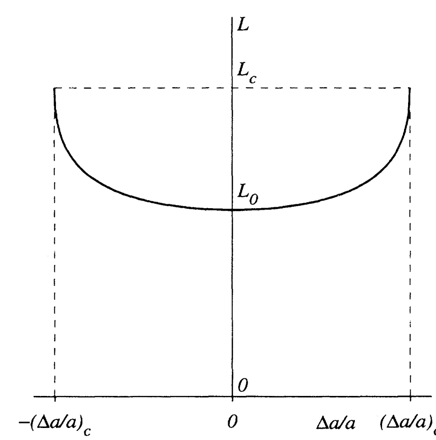

FIG. 5. Period of the metastable faceted structure versus lattice mismatch (linear theory of elasticity).

and the equilibrium period of faceting is no longer an even function of $\Delta a/a$. This results in some asymmetry in the plot of Fig. 5. In the present paper we do not consider this situation, and we treat, as already noted, the simple case of equal elastic moduli of the epitaxial film and the substrate.

III. FACETED SURFACE WITH SMALL TILT ANGLE OF FACETS

The analytic evaluation of the elastic energy $E^{\rm surf}_{\rm elastic}$ is possible for a faceted surface with small tilt angle of facets φ. We consider systems, where both the substrate and the epitaxial film have at least orthorhombic Bravais lattices with symmetry planes (xy), (xz), (yz). Then the intrinsic strain tensor $\varepsilon^{(0)}_{ij}$, describing the lattice mismatch between the epitaxial film and the substrate, is diagonal in axes x,y,z. The general problem of the elasticity theory described by Eq. (13) reduces to the plane strain problem with the displacement vector $\mathbf{u}_i(\mathbf{r}) = (u_x(x,z);0;u_z(x,z))$. This situation includes, particularly, important cases of cubic crystals where the axes x, y, z are $[1\bar{1}0]$, $[110]$, and $[001]$ directions [like in AlAs (Ref. 45)], or $[110]$, $[001]$, and $[1\bar{1}0]$ directions [like in TaC (Ref. 12)], or $[100]$, $[010]$, and $[001]$ directions [like in the system of strained Ge islands on Si (Refs. 15 and 16)].

We will consider below $E^{\rm surf}_{\rm elastic}$ from Eq. (27) up to quadratic terms in φ. The effective "surface-stress forces" P_i acting at crystal edges are equal to the difference of corresponding components of the intrinsic surface-stress tensor of neighboring facets (Fig. 2); for the symmetric profile one gets $P_x = 0$, $P_z = \mp 2\tau\sin\varphi$. The effective force P_z for small angles of faceting φ is of the order of $P_z = 2\tau\sin\varphi \sim \varphi$. The component n_x of the normal vector to the surface is equal to $n_x = \mp\sin\varphi \sim \varphi$. Therefore, the vector $w_i(\mathbf{r})$ is of the order of φ. After transformations presented in Appendix B, we obtain the elastic energy $E^{\rm surf}_{\rm elastic}$ as follows:

$$E^{\rm surf}_{\rm elastic} = -\left(\tau_{xx}\varepsilon^{(0)}_{xx} + \tau_{yy}\varepsilon^{(0)}_{yy}\right) + \frac{1}{2L_x}\int\!\!\int dx dx' P_z(x) G^{(0)}_{zz}(x-x';0,0) P_z(x') - \frac{1}{L_x}\int\!\!\int dx dx' P_z(x) G^{(0)}_{zx}(x-x';0,0)\widetilde{\sigma_{xx}} n_x(x') + \frac{1}{2L_x}\int\!\!\int dx dx' \widetilde{\sigma_{xx}} n_x(x) G^{(0)}_{xx}(x-x';0,0)\widetilde{\sigma_{xx}} n_x(x') . \quad (33)$$

Since the Green's tensor in the zeroth order in $\nabla\zeta(x)$ depends on $(x-x')$, it is convenient to use the Fourier transformation and to express $\zeta(x)$, $n_x(x)$, $P_z(x)$ as Fourier series. The Fourier expansion of the symmetric sawtooth profile shown in Fig. 3 is

$$\zeta(x) = \frac{8\zeta_0}{\pi^2}\sum_{m=0}^{\infty}\frac{1}{(2m+1)^2}\cos\left((2m+1)\frac{2\pi x}{L}\right). \quad (34)$$

Substituting the Fourier expansion of $\zeta(x)$ from Eq. (34) and corresponding expansions of $n_x(x) = -\nabla\zeta(x)$ and $P_z(x) = \tau\nabla^2\zeta(x)$, as well as the Fourier transform of the Green's tensor $\widetilde{G_{ij}}^{(0)}(k_x;0,0)$ from Eq. (C1) into Eq. (33), one gets the surface contribution into the elastic energy up to the order of φ^2.

To evaluate the short-range energy of crystal edges in the case of small tilt angles, the following note should be given. 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 $(a/L_T)^2 \sim \varphi^2$.[31] This implies that energies of edges are equal to $\eta^+(\varphi) = \xi^+\varphi^2$, $\eta^-(\varphi) = \xi^-\varphi^2$, $\eta(\varphi) = \eta^+(\varphi) + \eta^-(\varphi) = (\xi^+ + \xi^-)\varphi^2$, where ξ^+, ξ^- do not depend on φ. Then the total surface energy per unit area of the substrate is equal to

$$E^{\rm surf}_{\rm elastic} = \varepsilon(\varphi)\left(1+\frac{\varphi^2}{2}\right) - \left[\tau_{xx}(\varphi)\varepsilon^{(0)}_{xx} + \tau_{yy}(\varphi)\varepsilon^{(0)}_{yy}\right] + \varphi^2\left[\frac{\xi}{L} - \frac{4(\alpha_1+\alpha_2)\sqrt{\widetilde{c_{11}}\widetilde{c_{33}}}}{\pi(\widetilde{c_{11}}\widetilde{c_{33}} - \widetilde{c_{13}}^2)}\frac{\tau_{xx}(\varphi)^2}{L}\ln\frac{L}{a} - \tau_{xx}(\varphi)\frac{\widetilde{\sigma_{xx}}}{\sqrt{\widetilde{c_{11}}\widetilde{c_{33}}} + \widetilde{c_{13}}} - \frac{7Z(3)}{4\pi^3}\frac{(\alpha_1+\alpha_2)\widetilde{c_{33}}}{\widetilde{c_{11}}\widetilde{c_{33}} - \widetilde{c_{13}}^2}\widetilde{\sigma_{xx}}^2 L\right] . \quad (35)$$

Here, elastic moduli are given in the Voigt notation defined with respect to the reference axes x, y, z: $\widetilde{c_{11}} = \lambda_{xxxx}$, $\widetilde{c_{13}} = \lambda_{xxzz}$, $\widetilde{c_{33}} = \lambda_{zzzz}$, $\widetilde{c_{55}} = \lambda_{xzxz}$; α_1, α_2 are dimensionless attenuation coefficients of the static analogs of Rayleigh waves, they are defined in Appendix C, $Z(3) = 1.202$ is the Riemann ζ function. We do not expand in powers of φ the surface energy $\varepsilon(\varphi)$ and the intrinsic surface stress $\tau(\varphi)$, which have cusps as functions of φ.

Now we apply our results to the particular case of the AlAs epitaxial film on the (001) substrate. It was found by Mirin *et al.*[45] that the high-temperature growth of thick AlAs(001) layers results in the surface corrugation along the $[1\bar{1}0]$ direction. To analyze this structure, one should substitute $\varepsilon^{(0)}_{ij} = (\Delta a/a)\delta_{ij}$ into Eqs. (17,18,20), solve these equations, substitute $\widetilde{\sigma_{xx}}$ into Eq. (30), and express elastic moduli as follows: $\widetilde{c_{11}} = \frac{1}{2}(c_{11} + c_{12} + 2c_{44})$, $\widetilde{c_{13}} = c_{12}$, $\widetilde{c_{33}} = c_{11}$, $\widetilde{c_{55}} = c_{44}$ (here, c_{11}, c_{12}, c_{44} are elastic moduli in the Voigt notation defined with respect to cubic axes of the crystal). Then the first, the second, and the fourth L-dependent terms in rectangular parentheses on the right hand side of Eq. (35) may be rewritten in a way similar to Eq. (31). The critical value of the lattice mismatch is then equal to

$$\left(\frac{\Delta a}{a}\right)_c = \frac{2\sqrt{2}\pi}{\sqrt{7e\,Z(3)}} f(\varphi) \frac{c_{11}}{(c_{11}+2c_{12})(c_{11}-c_{12})} \times \left[\frac{c_{11}+c_{12}+2c_{44}}{2c_{11}}\right]^{1/4} \frac{\tau_{xx}(\varphi)}{L_0} . \quad (36)$$

Here, $f(\varphi)$ is the numerical function of the tilt angle φ, $f(0) = 1$. To obtain $f(\varphi)$ for finite φ, we have applied the finite element method[46] for solving the plane strain problem of the continuum theory of elasticity. The method is based on the variational principle[47] which implies minimization of the elastic strain energy given in Eq. (12). Note that both the heterophase structure displayed in Fig. 3 and the distribution of effective external forces are periodic and contain 2 mirror planes per each period. Therefore, we have solved the problem for a half of the period, the cell being displayed in Fig. 6. The finite element model of the cell consisted of 480 quadratic eight-noded quadrilateral isoparametric elements of Serendipity family,[46] the total number of degrees of freedom was 3058.

To solve the plane strain problem of the elasticity theory, we have used the homemade software for the finite element analysis.[48] We have imposed symmetric boundary conditions ($u_x = 0$, $\partial u_z/\partial x = 0$) on mirror planes $x = 0$ and $x = L/2$, zero boundary conditions in the bulk [$u_i = 0$ at $z = -(h+h_1)$], and have calculated the elastic strain energy. We have found that if the number of finite elements N_{FE} changes from 240 to 480, the strain energy changes less than by 0.2%. The strain energy has been obtained as a quadratic function of $(\Delta a/a)$ and τ in the form of Eq. (30). Since the term proportional to τ^2 depends logarithmically on a microscopic cutoff parameter a, we have performed calculations for different values of L. Interpolation of numerical results in accordance with Eq. (30) allows us to get the correct strain energy with the logarithmic accuracy.

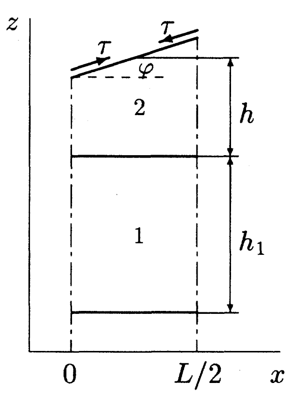

FIG. 6. The cell used in numerical calculations by the finite element method. One-half of the period of the corrugated heterostructure is displayed. "1" denotes the substrate; "2" denotes the epitaxial film; dashed-dotted lines denote mirror planes $x = 0$ and $x = L/2$ of the structure.

This numerical procedure has been applied for the particular AlAs(001) structure corrugated in the [1$\bar{1}$0] direction. The function $f(\varphi)$ which enters Eq. (36), is found to be smooth function of the tilt angle. It varies from 1 for $\varphi = 0$ to 1.25 for $\varphi = 45°$. Although there is no exact values of τ for AlAs in present literature, one may use for an order-of-magnitude estimation the values of the components of the intrinsic surface-stress tensor calculated for Si(001) (2×1) surface with symmetric dimers,[35,49] for Si(001) (2×1) surface with buckled dimers,[50] for GaAs(001) As-terminated (2×4) surface with a missing dimer row of As.[51] The estimation yields $\tau \sim 100$ meV/Å^2. For the faceted AlAs(001) surface with the characteristic periodicity 1800 Å observed in Ref. 45, Eq. (36) gives $(\Delta a/a)_c \approx 1.5 \times 10^{-4}$. The lattice mismatch between the AlAs epitaxial film and the GaAs substrate is, in fact, very small (4×10^{-4} at the temperature of the epitaxy 650 °C). Nevertheless, it exceeds the critical value $(\Delta a/a)_c$. Therefore, the observed faceting is governed by kinetic mechanism which results in irregular shape of the surface.

IV. NONLINEAR MODEL OF A STRAIN-DEPENDENT FACETING

The period of the faceted structure without lattice mismatch determined by the minimum of $E^{\text{surf}}_{\text{elastic}}$ from Eq. (35) is equal to

$$L_0 = a \exp(Q+1) , \quad (37)$$

where

$$Q = \frac{\pi\xi(\widetilde{c_{11}}\widetilde{c_{33}} - \widetilde{c_{13}}^2)}{4(\alpha_1+\alpha_2)\sqrt{\widetilde{c_{11}}\widetilde{c_{33}}}\,\tau(\varphi)^2} . \quad (38)$$

Parameters entering Eq. (38) are intrinsic parameters of the crystal. External strain being applied to the system, these parameters [namely, the short-range energy of the crystal edge $\eta(\varphi) = \xi\varphi^2$, the intrinsic surface stress $\tau(\varphi)$, elastic moduli $\widetilde{c_{ij}}$] change with strain. Due to the exponentially steep dependence of L_0 on Q, even small changes of these parameters may cause a dramatic effect on the period of faceting.

The steepest change with the strain is expected for the short-range energy of the crystal edge $\eta(\varphi) = \xi\varphi^2$. Indeed, this energy depends on the electronic structure near the edge atoms. This structure shows dramatic lability with respect to external perturbation (thus, the edge atoms in covalent semiconductors have the maximum number of electronic bonds which undergo rebonding). An example of this lability is given by the dependence of local energies and of the values of force dipoles of single-atomic and double-atomic steps on the Si(001) surface. The dependence of the values of force dipoles on the surface stress was found for all types of steps on Si(100) surface by Poon *et al.*[52]

Moreover, microscopic model calculations performed by Gilmer for Si(001) surface under external stress[53] yield a dramatic dependence of the local energy λ_0^{SB} of single-atomic B steps (SB steps) on external stress. The value of λ_0^{SB} for the stress-free Si(100) surface inferred from experiment by Swartzentruber *et al.*[54] is 24 meV/Å, the theoretical value is 17 meV/Å.[55] This energy is lowered by 20 meV/Å under the compressive strain of 1% and exhibits linear strain dependence in the region of strains from −2% to 2%.[53]

To give an insight on possible nonlinear effects in the strain-dependent faceting, we consider here the simple model. The factor Q in Eq. (38) which should depend on a local strain in the vicinity of crystal edges, is approximated by a model linear function of the overall lattice mismatch Δa as follows:

$$Q(\Delta a) = Q\left[1 - \gamma\left(\frac{\Delta a}{a}\right)\right]. \qquad (39)$$

Comparing Eq. (39) with the strain dependence of the energy of SB steps on Si(001), we may assume that the coefficient γ can be as large as 50 − 100, mainly due to the dependence of the short-range energy of crystal edges on strain. Substituting Q from Eq. (39) into Eq. (37) and then into Eq. (31), we may write down the L-dependent part of the surface energy as the function of L/L_0, this function being governed now by 2 control parameters:

$$\mu = \frac{(\Delta a/a)}{(\Delta a/a)_c}, \qquad (40)$$

$$p = \gamma Q\left(\frac{\Delta a}{a}\right)_c. \qquad (41)$$

Here, μ is the relative lattice mismatch defined in units of the critical lattice mismatch of the linear theory; p is the dimensionless parameter of nonlinearity. The L-dependent part of the surface energy from Eq. (31) now takes the form

$$E(L) = E_0\left[-\frac{L_0}{L}\left(\ln\frac{eL}{L_0} + p\mu\right) - \frac{1}{2e}\mu^2\frac{L}{L_0}\right]. \qquad (42)$$

The local minimum of this function gives the period of the metastable faceted structure. The value of L versus the relative lattice mismatch μ for different values of the dimensionless parameter of nonlinearity (in the case $p > 0$) is presented in Fig. 7. It is seen that the dependence of L on $\mu \equiv (\Delta a/a)/(\Delta a/a)_c$ is no longer an even function. The period L may be smaller than its value L_0 in the absence of the lattice mismatch. The curve $L(\mu)$ consists of 2 branches (the second branch appears in the region of very large μ which is usually unphysical) if $p < 1/e$, and is a monotonously decreasing function which consists of one branch for $p > 1/e$.

The approach of the macroscopic faceting is valid as long as the depth of the surface corrugation is much larger than the lattice constant, $\frac{1}{2}L\tan\varphi \gg a$. If this condition does not hold, the surface becomes apparently

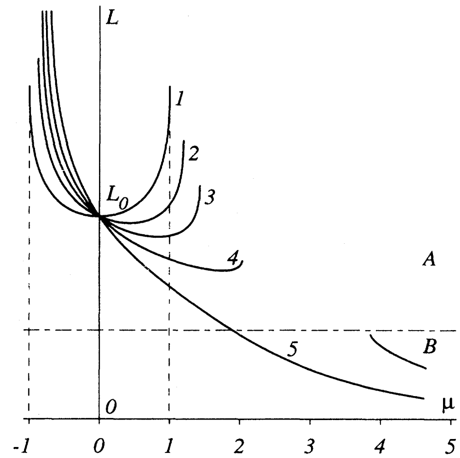

FIG. 7. Period of the metastable faceted structure versus lattice mismatch in the nonlinear model of strain-dependent faceting [$\mu = (\Delta a/a)/(\Delta a/a)_c$ is the relative value of the lattice mismatch]. Dimensionless parameter of nonlinearity is equal to (1) $p = 0$; (2) $p = 0.15$; (3) $p = 0.25$; (4) $p = 0.35$; (5) $p = 0.5$. (a) The region of macroscopic faceting; (b) the region of microscopic surface reconstruction.

flat although microscopically reconstructed. The dashed-dotted line in Fig. 7 schematically separates these two regions.

It follows from Fig. 7 that nonlinear effects in the strain-dependent faceting are essential for $p \gtrsim 0.25$. Substituting of Q from Eq. (38) and $(\Delta a/a)_c$ from Eq. (36) into Eq. (41) yields the following estimation for p:

$$p = \gamma\ln\left(\frac{L_0}{ea}\right)\frac{2\tau}{YL_0}, \qquad (43)$$

where Y is the characteristic bulk elastic modulus. Using typical values of $Y \approx 800$ meV/Å^3, $\tau \approx 100$ meV/Å^2, $\gamma \approx 50$, one gets that $p = 0.25$ at L_0 =50 Å. This estimation separates the faceted surfaces with smaller periods where nonlinear effects are strong from those with larger periods, where faceting may be described by the linear theory of elasticity.

Experimental data of Tournié *et al.*[56] seem to be an example of nonlinear effects in strain-dependent faceting. The period of the faceted InAs(311) grown on the lattice-mismatched $Ga_{1-x}In_xAs$ decreases with the increase of $|\Delta a|$ ($\Delta a > 0$), and then the surface becomes apparently flat. The similar decrease of the period with $|\Delta a|$ was observed for GaAs(311) on lattice-mismatched $Ga_{1-x}In_xAs$ (here $\Delta a < 0$). These results are in reasonable qualitative agreement with our nonlinear model of strain-dependent faceting if one assumes that the parameter of nonlinearity γ is positive for InAs(311) and negative for GaAs(311). Since nonlinear effects are very sensitive to the particular electronic structure on surfaces and at crystal edges, the fact that γ may have opposite signs for GaAs and InAs seems to be understandable.

There is a peculiarity of experimental data of Ref. 56 to be taken into account. It is a thick (relaxed) InAs/GaAs layer grown on GaAs(311) substrate, which was considered as completely unstrained InAs(311). However, thick relaxed lattice-mismatched layers are known to contain a set of misfit dislocations and anisotropic residual stresses.[57] Thus, the relaxed InAs/GaAs system can hardly be considered as the reference point for the faceting without external stress. Moreover, periods of faceted structures on a lattice-matched GaAs/GaAs(311) system and on a relaxed $GaAs/Ga_{0.47}In_{0.53}As(311)$ system were found to be slightly different (32 Å and 39 Å). This implies that an alternative interpretation of experimental data of Ref. 56, which includes small residual stress in the epilayer is possible as well. The (311) surface of an InAs monocrystal would be a more appropriate surface to observe the intrinsic faceting of the InAs(311) surface.

V. FACETING OF A LOADED SAMPLE

We study, in the present section, the elastic energy of a sample where its upper surface undergoes faceting, and external load $\sigma_{ab}^{\rm ext}$, $(a,b = x,y)$ is applied. The elastic energy contains bulk ($E_{\rm elastic}^{\rm bulk}$) and surface ($E_{\rm elastic}^{\rm surf}$) contributions, the former depends on particular boundary conditions on lateral and bottom surfaces, the latter is not sensitive to them. Before we separate these two contributions, we need to formulate the problem for a whole sample.

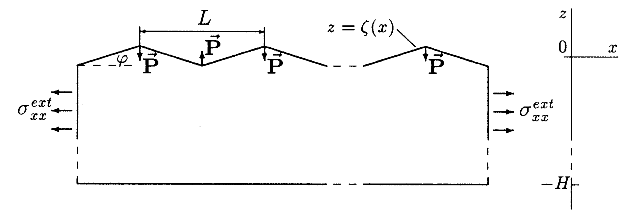

FIG. 8. Faceted surface of a loaded sample.

We consider the particular situation where an external in-plane load is applied uniformly to a lateral surface (Fig. 8), and the bottom surface is free and does not undergo faceting. The boundary conditions read, for this case,

$$\sigma_{ij} n_j|_{z=\zeta(x)} = P_i(\mathbf{r})\,, \tag{44a}$$

$$\sigma_{ib} n_b|_{\substack{\rm lateral\\ \rm surface}} = \delta_{ia}\sigma_{ab}^{\rm ext}\,, \tag{44b}$$

$$\sigma_{iz}|_{z=-H} = 0\,, \tag{44c}$$

and the displacement vector obeys the set of coupled homogeneous equations in the bulk of the sample, $\lambda_{ijlm}\nabla_j\nabla_l u_m(\mathbf{r}) = 0$. The solution of these equations with the boundary conditions (44) gives the elastic energy per unit area of the reference flat surface as follows, $E_{\rm elastic} = E_{\rm elastic}^{\rm bulk} + E_{\rm elastic}^{\rm surface}$, where $E_{\rm elastic}^{\rm bulk} = -\frac{1}{2}\sigma_{ab}^{\rm ext}\widetilde{\varepsilon_{ab}}h$, and

$$E_{\rm elastic}^{\rm surf} = -\left(\tau_{xx}\widetilde{\varepsilon_{xx}} + \tau_{yy}\widetilde{\varepsilon_{yy}}\right) \tag{45a}$$

$$-\widetilde{\varepsilon_{xz}}\frac{1}{L_x}\int dx P_x(x)\zeta(x) - \frac{\widetilde{\varepsilon_{zz}}}{2}\frac{1}{L_x}\int dx P_z(x)\zeta(x) \tag{45b}$$

$$+\frac{1}{2L_x}\int\int dl dl' P_i(x) G_{ij}(x,\zeta(x);x',\zeta(x'))P_j(x') \tag{45c}$$

$$-\frac{1}{L_x}\int\int dl dl' P_i(x) G_{ij}(x,\zeta(x);x',\zeta(x'))\sigma_{jx}^{\rm ext} n_x(x') \tag{45d}$$

$$+\frac{1}{2L_x}\int\int dl dl' \sigma_{ix}^{\rm ext} n_x(x) G_{ij}(x,\zeta(x);x',\zeta(x'))\sigma_{jx}^{\rm ext} n_x(x') \tag{45e}$$

$$-\widetilde{\varepsilon_{xx}}\frac{1}{L}\int_0^L dx\; x P_x(x) - \widetilde{\varepsilon_{xj}}\frac{1}{L}\int_0^L dx\; x\widetilde{\sigma_{jx}^{\rm ext}} n_x(x)\,, \tag{45f}$$

(here $\widetilde{\varepsilon_{ij}} \equiv S_{ijab}\sigma_{ab}^{\rm ext}$, S_{ijlm} being the tensor of elastic compliances). The terms from Eqs. (45a,b,c,d,e) are similar to those of Eqs. (27a,b,c,d,f), respectively. The two terms from Eq. (45f) depend on particular geometry of lateral edges of the sample. However, these contributions defined per unit area of the nominal flat surface, do not depend on L.

Thus, the elastic energy of a loaded sample with a faceted top surface contains similar contributions as $E_{\rm elastic}$ of an epitaxial film on a lattice-mismatched substrate considered in Sec. II. Therefore, the total surface energy may be written in the schematic form similar to Eq. (31):

$$E(L) = E_0\left[-\frac{L_0}{L}\ln\frac{eL}{L_0} - \frac{1}{2e}\left(\frac{\sigma_{xx}^{\rm ext}}{\sigma_c}\right)^2\frac{L}{L_0}\right], \tag{46}$$

(σ_c being a critical value of external load).

If a small load $\sigma_{xx}^{\rm ext} < \sigma_c$ is applied to the faceted surface, transition to the stable state may be kinetically forbidden. Then the surface stays in the metastable faceted state, and the period of the faceting increases with the load. Applying a load larger than the critical value σ_c results in the breakdown of formation of metastable faceted structures. The metastable state then disappears, and the surface undergoes transition to the stable state which is determined by the particular geometry of the sample. If the period of the faceted structure without load is sufficiently small ($L_0 \lesssim 50$ Å) then the stress dependence of the period may be described by a nonlinear model presented in Sec. IV.

The possibility of applying an external load, which could be varied in a controlled way in a wide scale corresponding to deformations from 10^{-4} to 10^{-2} was proved experimentally by Men *et al.*[34] Therefore, we expect that experimental observations of the dependence of faceting on external stress are possible for loaded samples, too.

VI. CONCLUSIONS

We have studied theoretically the effect of externally applied stress on the type of faceting, where the faceting of the surface initially occurs *without* any external stress. We have considered in detail the technologically relevant way of applying external stress, namely, the heteroepitaxial growth on a lattice-mismatched substrate. We have found that there exists a metastable state of the heterophase system which is a continuous epitaxial film with periodically corrugated top surface. The period of the surface corrugation L varies with the lattice mismatch $\Delta a/a$, and two different scenarios of the dependence of L on $\Delta a/a$ are possible.

It the period of surface corrugation without external stress L_0 exceeds the order of ≈ 50 Å, then the dependence of the period L on the lattice mismatch may be described in the frame of the linear theory of elasticity. Then the period of surface corrugation increases both for tensile and compressive mismatch-induced strain. The dependence of L on $|\Delta a/a|$ gives a possibility to control the period of surface corrugation by varying $|\Delta a/a|$. If the mismatch is larger than a certain critical value $(\Delta a/a)_c$, then the metastable state disappears, which means the breakdown of formation of metastable faceted structures. For the surfaces with small tilt angle of facets φ, the critical lattice mismatch is determined by Eq. (36). Numerical tests performed for large angles φ indicate that $(\Delta a/a)_c$ depends only weakly on the tilt angle of facets. Since the order of magnitude estimation for $\tau \sim 100$ meV/Å^2 is valid for a large class of solids, one may use Eq. (36) to evaluate the critical value of the lattice mismatch for different faceted surfaces. For faceted surfaces with periods $L_0 \sim 1000 - 2000$ Å, the critical lattice mismatch is $(\Delta a/a)_c \sim 10^{-4}$. For faceted surfaces with periods $L_0 \sim 20 - 30$ Å,[12,13] the critical lattice mismatch is equal to $(\Delta a/a)_c \approx 5 \times 10^{-3}$.

In the case where the period of the faceted structure *without external stress* is $L_0 \lesssim 50$ Å, the dependence of L on Δa is determined by nonlinear elastic effects. Then the period L increases for one sign of Δa up to the breakdown of formation of metastable faceted structures and decreases for another sign of Δa, where the macroscopic faceting transforms gradually into a microscopic surface reconstruction and the surface becomes apparently flat. This situation seems to occur in heterophase systems GaAs/InAs(311) and InAs/GaAs(311).[56] Note that the characteristic length of facets corresponding to the crossover from linear model to nonlinear one is very sensitive to the particular orientation of the surface. Therefore, the strain dependence of the period L for a class of faceted structures where $L_0 \sim 20 - 50$ Å, may be very different from one material to another and from one surface orientation to another.

As a summary, we have considered the effect of externally applied stress on surface faceting. We have shown that the variation of the lattice mismatch provides a powerful tool to tune surface periodicity in a controlled way.

ACKNOWLEDGMENTS

The work was supported, in different parts, by the International Science Foundation, by the French Government, and by the Volkswagen Stiftung. V.A. Sh. is grateful to C.A. Sébenne for valuable discussions and for the hospitality provided by the Laboratoire de Physique des Solides during his stay in Paris.

APPENDIX A

It is possible to obtain the dependence of all coefficients A, B, C in Eq. (29) on the period of faceting L before solving Eq. (23) for the Green's tensor, just from simple scaling arguments. The only term $\sim P^2$ in Eq. (27) is that of Eq. (27c). The Green's tensor $G_{ij}(\mathbf{r}, \mathbf{r}')$ for the two-dimensional problem of the elasticity theory depends logarithmically on the distance, $G \sim \ln|\mathbf{r} - \mathbf{r}'|$. Effective surface-stress forces P_i are concentrated at crystal edges, the total force per period vanishes. Therefore, the interaction of far edges is compensated, and that of several neighboring edges dominates in Eq. (27c). Thus, the energy per one period is $\sim \ln L$. Correspondingly, the energy per unit surface area is $\sim \ln L/L$ [see, also Ref. 28)]. Since this energy term is the energy of elastic relaxation of the faceted surface, it is negative, and $A(L) \sim -\ln L/L$.

The contributions to $B(L)$ in Eq. (29) come from terms (27a,27b,27d,27e,27g). The term (27d) can be rewritten as follows:

$$-\frac{L_y}{2} \int dx P_i(x) w_i^M(x, \zeta(x)) \,. \tag{A1}$$

Here the vector $w_i^M(x,z)$, defined by $w_i^M(x,z) = \int dx' G_{ij}(x,z;x',\zeta(x'))\widetilde{\sigma_{jx}} n_x(x')$, satisfies the set of coupled homogeneous equations (21) and the boundary conditions

$$\lambda_{ijlm} n_j(x) \frac{\partial}{\partial r_l} w_m(x,z)\bigg|_{z=\zeta(x)} = -\widetilde{\sigma_{ix}} n_x(x) \,. \tag{A2}$$

We note here that both homogeneous equations (21) and boundary conditions (A2) remain invariant with respect to rescaling:

$$\mathbf{r} \to \widetilde{\mathbf{r}} = \beta \mathbf{r}\,, \qquad \zeta(\widetilde{x}) = \beta\zeta(x)\,, \qquad w_i^M(\widetilde{\mathbf{r}}) = \beta w_i^M(\widetilde{\mathbf{r}})\,. \tag{A3}$$

Then the energy (A1) calculated per one period of the faceted structure scales proportional to β, i.e., the energy is proportional to L. Therefore, the energy per unit surface area is L independent.

Due to the reciprocity properties of the Green's tensor $[G_{ij}(x',z';x,z) = G_{ji}(x,z;x',z')]$, the term from Eq. (27e) can be considered in the same way. This proves that the coefficient $B(L)$ in Eq. (29) does not depend on L.

The similar scaling arguments applied to the term (27f) in $F^{\rm surf}_{\rm elastic}$ show that the energy per one period L scales as β^2, i.e., is proportional to L^2. Therefore, the energy per unit surface area, i.e., the coefficient $C(L)$ in Eq. (29), is proportional to L.

APPENDIX B

To simplify the expression (27) for the elastic energy $E^{\rm surf}_{\rm elastic}$ in the case of small tilt angle of facets φ and to calculate the lowest-order in φ term in $E^{\rm surf}_{\rm elastic}$, we note that the two terms of Eqs. (27e,f) may be written as $\frac{1}{2}\int dx \sigma^{(0)}_{ij} n_j(x) w_i(x;\zeta(x))$. To proceed, we consider the quantity

$$\begin{aligned}\int dx\ \widetilde{\sigma_{ij}} n_j(x) w_i(x;\zeta(x)) &= \int dx\ \lambda_{iblm}\widetilde{\varepsilon_{lm}} n_b(x) w_i(x;\zeta(x)) \\ &\quad + \int dx\ \lambda_{izlm}\widetilde{\varepsilon_{lm}} n_z(x) w_i(x;\zeta(x)) \\ &\quad - \int dx\ \sigma^{(0)}_{ij} n_j(x) w_i(x;\zeta(x))\,.\end{aligned} \tag{B1}$$

To calculate the contribution of the order of φ^2 into Eq. (B1) it is sufficient to substitute $n_b(x) = -\nabla_b\zeta(x)$ into the first term on the right hand side of Eq. (B1) and to integrate it by parts. In the second term of Eq. (B1) one should replace $n_z(x)$ by 1 and expand $w_i(x;\zeta(x)) = w_i(x;0) + \zeta(x)\frac{\partial w_i(x;0)}{\partial z}$. Then Eq. (B1) is transformed into

$$\begin{aligned}\int dx\ \widetilde{\sigma_{ij}} n_j(x) w_i(x;\zeta(x)) &= 2\int dx\ \zeta(x)\,\widetilde{\varepsilon_{bz}}\lambda_{bzij}\left.\frac{\partial w_i}{\partial r_j}\right|_{z=\zeta(x)} \\ &\quad + \int dx\ \zeta(x)\,\widetilde{\varepsilon_{zz}}\lambda_{zzji}\left.\frac{\partial w_i}{\partial r_j}\right|_{z=\zeta(x)} \\ &\quad - \int dx\ \sigma^{(0)}_{ij} n_j(x) w_i(x;\zeta(x))\,.\end{aligned} \tag{B2}$$

After substituting Eq. (22) into the first and the second term of Eq. (B2), this equation is reduced to

$$\begin{aligned}\int dx\ \widetilde{\sigma_{ij}} n_j(x) w_i(x;\zeta(x)) &= 2\int dx\ \zeta(x)\,\widetilde{\varepsilon_{bz}} P_b(x) \\ &\quad + \int dx\ \zeta(x)\,\widetilde{\varepsilon_{zz}} P_z(x) \\ &\quad - \int dx\ \sigma^{(0)}_{ij} n_j(x) w_i(x;\zeta(x))\,.\end{aligned} \tag{B3}$$

Now we express the vector $w_i(x;\zeta(x))$ in terms of the Green's tensor $G_{ij}(\mathbf{r};\mathbf{r}')$ and substitute Eq. (B3) into Eqs. (27b,e,f). Within the required accuracy of φ^2 it is sufficient to use the Green's tensor $G_{ij}(x,\zeta(x);x',\zeta(x'))$ in the zeroth order with respect to $\zeta(x)$, i.e., to use the Green's tensor of the semi-infinite medium with the flat surface, which depends on the relative distance along the surface, $G_{ij}(x,\zeta(x);x',\zeta(x')) \approx G^{(0)}_{ij}(x-x';0,0)$. Then the elastic energy $E^{\rm surf}_{\rm elastic}$ reduces to the form of Eq. (33).

APPENDIX C

The Green's tensor $G^{(0)}(\mathbf{r};\mathbf{r}')$, can be easily calculated in the zeroth order in $\nabla\zeta(\bar{x})$ for a crystal of at least orthorhombic symmetry. To calculate $F^{\rm surf}_{\rm elastic}$ from Eq. (21) one needs the Fourier transform of the Green's tensor, $\widetilde{G^{(0)}_{ij}}(k_x;k_y=0;z,z'=0)$. Equation (21) reduces for these components into two sets of two coupled equations each. A straightforward solution of these equations yields

$$\widetilde{G^{(0)}_{xx}}(k_x;k_y=0;z=0,z'=0) = -\frac{(\alpha_1+\alpha_2)}{|k_x|}\frac{\widetilde{c_{33}}}{\left(\widetilde{c_{11}}\widetilde{c_{33}}-\widetilde{c_{13}}^2\right)}\,, \tag{C1a}$$

$$\widetilde{G^{(0)}_{xz}}(k_x;k_y=0;z=0,z'=0) = -\frac{i\,{\rm sgn}(k_x)}{|k_x|}\frac{1}{\sqrt{\widetilde{c_{11}}\widetilde{c_{33}}}+\widetilde{c_{13}}}\,, \tag{C1b}$$

$$\widetilde{G^{(0)}_{zx}}(k_x;k_y=0;z=0,z'=0) = -\frac{i\,{\rm sgn}(k_x)}{|k_x|}\frac{1}{\sqrt{\widetilde{c_{11}}\widetilde{c_{33}}}+\widetilde{c_{13}}}\,, \tag{C1c}$$

$$\widetilde{G^{(0)}_{zz}}(k_x;k_y=0;z=0,z'=0) = -\frac{(\alpha_1+\alpha_2)}{|k_x|}\frac{\sqrt{\widetilde{c_{11}}\widetilde{c_{33}}}}{\left(\widetilde{c_{11}}\widetilde{c_{33}}-\widetilde{c_{13}}^2\right)}\,. \tag{C1d}$$

Here, dimensionless attenuation coefficients of static analogs of Rayleigh waves α_1, α_2 are determined by the equation

$$\widetilde{c_{33}}\widetilde{c_{55}}\alpha^4 + \left(\widetilde{c_{13}}^2 + 2\widetilde{c_{13}}\widetilde{c_{55}} - \widetilde{c_{11}}\widetilde{c_{33}}\right)\alpha^2 + \widetilde{c_{11}}\widetilde{c_{55}} = 0\,, \tag{C2}$$

where $\mathrm{Re}\alpha_{1,2} > 0$. For a cubic crystal with the z axis parallel to the [001] direction of the crystal and the x axis parallel to either [100] or [110] direction, the Green's tensor from Eq. (C1) coincides with that from Ref. 58.

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