

# Enhanced formation of nanowires and quantum dots on dislocated substrates

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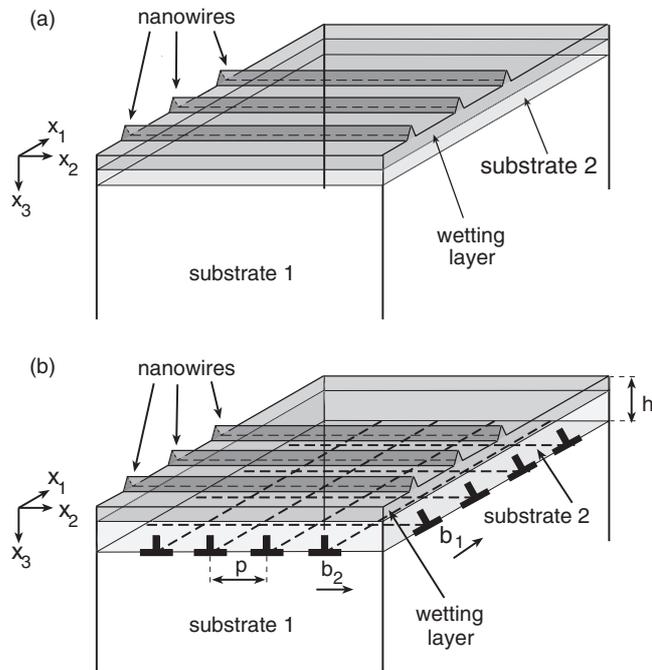
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## Abstract

A new mode of enhanced growth of semiconductor nanowires and quantum dots on mismatched substrates is suggested and theoretically examined. This mode is based on the effects of misfit dislocations located in a composite two-layer substrate on the epitaxial growth on the substrate surface. It is shown that stress fields of such dislocations are capable of essentially enhancing the formation of nanowires and quantum dots on dislocated substrates, compared to the conventional case of non-dislocated substrates. In particular, in certain ranges of parameters of heteroepitaxial systems, the growth of quantum dots and nanowires on non-dislocated substrates is forbidden, while their growth on dislocated substrates with the same parameters is energetically favourable.

## 1. Introduction

The rapidly growing scientific and technological interest in semiconductor nanowires and nano-islands (quantum wires and dots) arise from the unique properties associated with their nanoscale structure; see, e.g., [1–22]. In particular, the phenomenon of nanowire and quantum dot formation in mismatched heteroepitaxial structures attracts much attention as a manifestation of fundamental nanoscale and interface effects in solids, as well as a basis for a range of new nanotechnologies. The conditions of the formation of nanowires and quantum dots are among the most important issues that influence their structure, chemical compositions and thereby functional properties. The nanowires and quantum dots growing on either a substrate or a wetting layer represent the sources of stress fields due to a crystal-lattice misfit (geometric mismatch) between the substrate and nanowires or quantum dots. As a corollary, the formation and growth of nanowires and quantum dots are sensitive to stress distribution in the substrate. In this context, it is possible to control and design the formation of nanowires and quantum dots and their functional characteristics through manipulation of stress sources in the substrate.



**Figure 1.** Nanowires on a two-layer composite substrate. (a) Substrate does not contain dislocations. (b) Substrate contains a misfit dislocation network.

The effect of stress sources in the substrate on the spatial arrangement of nanowires and quantum dots has been investigated in a large number of theoretical (e.g., [7–12]) and experimental (e.g., [13–20]) works. However, we think that the presence of stress sources in the substrate may not only control the lateral arrangement of nanowires and quantum dots but also change the growth mode of the film on this substrate. In particular, we suppose that the formation of misfit dislocations in a composite substrate may change the growth mode of the film on this substrate from the Frank–van-der-Merwe mode (continuous film) to the Stranski–Krastanow one (nanowires or quantum dots on a wetting layer).

The main aim of this paper is to theoretically examine the influence of the stress fields of misfit dislocations located in a composite substrate on the formation of nanowires and quantum dots. We will demonstrate that the stress fields of these misfit dislocations are capable of essentially enhancing the formation of semiconductor nanowires and quantum dots on dislocated substrates, compared to the conventional case of non-dislocated substrates.

## 2. Epitaxial growth of nanowires on a dislocated substrate: model

First, let us examine the formation of nanowires on a dislocated substrate. We consider a model composite system consisting of a semi-infinite substrate 1 (phase 1), substrate 2 (phase 2) of finite thickness, and an epitaxial layer (phase 3) that grows on substrate 2 (figure 1). Substrates 1 and 2 as well as the epitaxial layer 3 are assumed to be isotropic solids characterized by the same values of the shear modulus  $\mu$  and the same values of the Poisson ratio  $\nu$ . The crystal lattices of the substrates 1 and 2 in the interphase (substrate 1/substrate 2) boundary plane are assumed to be square and have different lattice parameters  $a_{s1}$  and  $a_{s2}$ , respectively. In this

case, the two-dimensional misfit between the substrates exists which is characterized by the misfit parameter  $f = (a_{s1} - a_{s2})/a_{s1}$ . The misfit causes substrate 2 of finite thickness to be strained.

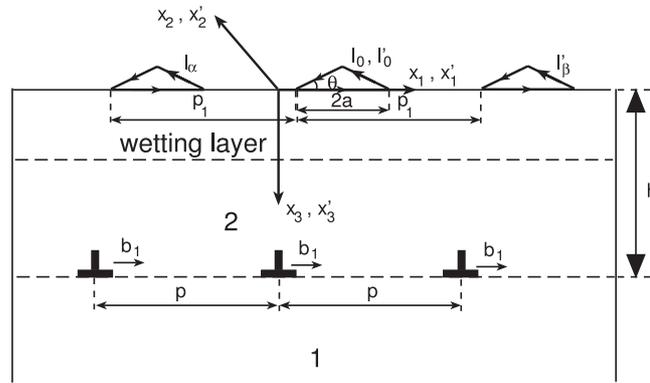
Following the theory of interphase boundaries in heteroepitaxial systems (see, e.g., [23–29]), the interphase boundary between substrate 1 and strained substrate 2 is in either a coherent (non-defected; see figure 1(a)) or a semi-coherent (defected; see figure 1(b)) state. If the thickness of substrate 2 is lower than some critical value, the interphase boundary is coherent (figure 1(a)). In doing so, the misfit between crystalline lattices of substrates 1 and 2 is accommodated completely by the uniform elastic straining of substrate 2 (figure 1(a)). As a result, the interatomic distances in phase 2 in the directions parallel to the interphase boundary become equal to the crystal parameter  $a_{s1}$  of phase 1. In the coordinate system  $(x_1, x_2, x_3)$  shown in figure 1, the directions parallel to the interphase boundary are  $x_1$  and  $x_2$ .

Let us consider the epitaxial layer (phase 3) growing as a continuous wetting layer on substrate 2 coherently matched with substrate 1 (figure 1(a)). In the framework of our model, we consider phase 3 characterized in its non-strained state by different crystal lattice parameters  $a_1$  and  $a_2$  in the directions  $x_1$  and  $x_2$ , respectively. During continuous growth of the wetting layer (phase 3) on substrate 2, the crystal lattice of the wetting layer uniformly strains to provide its matching with the crystal lattice of substrate 2. As a corollary, the interatomic distances in the wetting layer in the directions parallel to the interphase boundary plane become equal to the corresponding interatomic distances of phase 2, which in their turn are equal to  $a_{s1}$  (see above). Thus, the wetting layer shown in figure 1(a) is uniformly strained with the dilatational strains  $\varepsilon_{11} = f_1 = (a_{s1} - a_1)/a_{s1}$  and  $\varepsilon_{22} = f_2 = (a_{s1} - a_2)/a_{s1}$  in the directions  $x_1$  and  $x_2$ , respectively. Notice that the uniform strains in this wetting layer depend on the misfit between phases 1 and 3 but not between phases 2 and 3.

In some ranges of parameters  $f_1$  and  $f_2$  and other geometric and material characteristics, the epitaxial layer starts to grow in the form of parallel nanowires on the wetting layer (figure 1(a)), which are oriented along one of crystallographic axes; see, e.g., review [3]. When nanowires nucleate on the strained wetting layer, they also have to strain to provide the bonding of their atoms with the atoms of the strained wetting layer. That is, the wetting layer itself does not accommodate the misfits  $f_1$  and  $f_2$  between substrate 1 and the nanowires. In fact, the growth mode of the epitaxial layer changes from the Frank–van-der-Merwe mode (continuous wetting layer) to the Stranski–Krastanow one (nanowires on the wetting layer; see figure 1(a)) to accommodate in part the misfit strains in the epitaxial layer [3].

Now let us consider the situation where the thickness of phase 2 exceeds its critical value, causing the interphase boundary between substrates 1 and 2 to be semi-coherent (figure 1(b)). In this situation, the formation of misfit dislocations at the interphase boundary is energetically favourable, which effectively contributes to the accommodation of the misfit strains; see, e.g., [8–29]. For definiteness, in this paper we will focus our consideration on two orthogonal rows of edge misfit dislocations that form a square dislocation lattice with a period  $p$  at the interphase boundary between substrates 1 and 2 (figure 1(b)). The misfit dislocations belonging to the first and second dislocation rows are characterized by the Burgers vectors  $\mathbf{b}_1 = b_1 \mathbf{e}_1$  and  $\mathbf{b}_2 = b_2 \mathbf{e}_2$ , that are parallel with the boundary plane and shown in figure 1(b). Such regular rows of misfit dislocations have been observed experimentally [30–33] and have also exhibited their potential as stress sources causing a regular spatial arrangement of quantum dots on dislocated substrates [8, 9, 11, 16–20]. We think that the misfit dislocations at the interphase boundary between the substrates 1 and 2 (figure 1(b)) create stress fields that are able not only to affect spatial positions of nanowires but also to initiate or enhance their formation.

Let us examine the conditions at which the formation of nanowires on the composite substrate with misfit dislocations (figure 1(b)) is energetically favourable. Then we will



**Figure 2.** Row of nanowires on a substrate with misfit dislocations. (For clarity, the row of dislocations parallel to the axis  $x_2$  is not shown.)

compare these conditions with those of the energetically favourable formation of nanowires on a non-dislocated composite substrate (figure 1(a)). For definiteness, we consider a periodic model row (with a period  $p_1$ ) of identical nanowires growing on a thin wetting layer (figure 2). The nanowires have the shape of regular triangular prisms with base length  $2a$ , and contact angles  $\theta$  of their lateral surfaces with the free surface of the wetting layer. The misfit dislocation lines at the interphase boundary  $x_3 = h$  have the coordinates  $x_1 = mp$  and  $x_2 = np$ , where  $m$  and  $n$  are integers.

In general, nanowires growing on a dislocated substrate tend to nucleate at certain spatial positions determined by the elastic interaction between the nanowires and periodically ordered misfit dislocations. This effect is very similar to the well-known effect [8, 9, 11, 16–20] of misfit dislocations on spatial positions of quantum dots growing on a dislocated substrate. As with the case of quantum dots, after some algebra, one can find that the nanowires tend to be periodically arranged with a period  $p_1$  which is related to the period  $p$  of the misfit dislocation arrangement as follows:  $p_1 = p$  or  $p_1 = p/2$ , depending on the values of  $a/p$  and  $h/p$ . Figures 1(b) and 2 illustrate the simplest case of  $p_1 = p$ .

### 3. Energy characteristics of nanowires on a dislocated substrate

In order to determine the conditions of the nanowire formation, we will compare the energies that characterize the heteroepitaxial system in the two physical states, namely (a) the state where the epitaxial layer grows continuously (Frank–van der Merwe mode); and (b) the state where nanowires grow on the wetting layer (Stranski–Krastanow mode).

The difference  $\Delta W^{\text{nw}}$  between the energies of the system in states (b) and (a), per unit nanowire length and per nanowire, is as follows:

$$\Delta W^{\text{nw}} = W_{\text{rel}}^{\text{nw}} + \sum_{n=1}^{\infty} W_{\text{int}}^{\text{nw-nw}}(np_1) + W_{\text{int}}^{\text{ar1-nw}} + W_{\text{int}}^{\text{ar2-nw}} - W_{\text{int}}^{\text{ar1-f}} - W_{\text{int}}^{\text{ar2-f}} + \Delta W^{\text{surf}}. \quad (1)$$

Here  $W_{\text{rel}}^{\text{nw}}$  denotes the difference in the elastic self-energy of a nanowire and a continuous film fragment with the same volume;  $W_{\text{int}}^{\text{nw-nw}}(np_1)$  is the energy that characterizes interaction between two nanowires distant by  $np_1$  from each other;  $W_{\text{int}}^{\text{ar1-f}}$  and  $W_{\text{int}}^{\text{ar2-f}}$  are the energies of interaction of the first and second dislocation rows with the misfit stresses in a continuous film

fragment having length  $p_1$  and volume equal to that of one nanowire;  $\Delta W^{\text{surf}}$  is the surface energy change related to the formation of one nanowire on the wetting layer. In formula (1), we neglect the contribution of the surface stresses [3] and take into account that the misfit stresses in substrate 2 and the wetting layer do not interact with the stress fields created by nanowires.

The energy  $W_{\text{rel}}^{\text{nw}}$  is calculated using the shallow-facet approximation [3, 34–39] and may be written as:

$$W_{\text{rel}}^{\text{nw}} = -\frac{1}{2} \int_{-\infty}^{\infty} dx'_2 \oint_{l_0} \oint_{l'_0} n_i(\mathbf{x}') \sigma_{ij}^f(\mathbf{x}') G_{jk}(\mathbf{x}, \mathbf{x}')|_{x_3=x'_3=0} \sigma_{kl}^f(\mathbf{x}) n_l(\mathbf{x}) dl' dl. \quad (2)$$

Here  $l_0$  and  $l'_0$  are the contours surrounding the cross-section of a nanowire in the spaces  $(x_1, x_2, x_3)$  and  $(x'_1, x'_2, x'_3)$ , respectively (see figure 2),  $\mathbf{x}$  and  $\mathbf{x}'$  are points at the contours,  $\mathbf{n}(\mathbf{x})$  and  $\mathbf{n}(\mathbf{x}')$  are external normals to these contours,  $\sigma_{ij}^f$  is the stress field that would act in a planar film on a non-dislocated substrate in the absence of nanowires, and  $G_{jk}(\mathbf{x}, \mathbf{x}')$  is the Green tensor for an isotropic semi-infinite medium. The stress field  $\sigma_{ij}^f$  follows as:  $\sigma_{ij}^f = \sigma_0 \delta_{ij} (\delta_{i1} + \delta_{i2})$ , where  $\sigma_0^f = [2\mu(1+\nu)/(1-\nu)]f_e$ ,  $f_e = (f_1 + \nu f_2)/(1+\nu)$  is the effective misfit, and  $\delta_{ij}$  is the Kronecker delta.

The energy that characterizes the interaction between the two nanowires is effectively represented in a similar way as follows:

$$W_{\text{int}}^{\text{nw-nw}} = - \int_{-\infty}^{\infty} dx'_2 \oint_{l_\alpha} \oint_{l'_\beta} n_i(\mathbf{x}') \sigma_{ij}^f(\mathbf{x}') G_{jk}(\mathbf{x}, \mathbf{x}') \sigma_{kl}^f(\mathbf{x}) n_l(\mathbf{x}) dl' dl. \quad (3)$$

Here  $l_\alpha$  and  $l'_\beta$  are the contours that surround the interacting nanowires (see figure 2).

The substitution of the expressions [40] for the Green tensor  $G_{ij}$  into (2) and (3) yields:

$$W_{\text{rel}}^{\text{nw}} = - \frac{2(1-\nu)a^2 \ln 2 \sigma_{11}^{f^2} \tan^2 \theta}{\pi \mu}, \quad (4)$$

$$W_{\text{int}}^{\text{nw-nw}}(r) = - \frac{(1-\nu)\sigma_{11}^{f^2} \tan^2 \theta}{\pi \mu} g_2(a, r), \quad (5)$$

where

$$g_2(a, r) = 6r^2 \ln r - 4(r+a)^2 \ln(r+a) - 4(r-a)^2 \times \ln(r-a) + (r+2a)^2 \ln(r+2a) + (r-2a)^2 \ln(r-2a). \quad (6)$$

Formula (4) obtained here for  $W_{\text{rel}}^{\text{nw}}$  is different by a factor of 4/3 from the expression obtained in [34] using the Green functions for an infinite medium.

The energy  $W_{\text{int}}^{\text{ar1-nw}}$  that characterizes the interaction of the nanowire with the base centre line ( $x_1 = x_0, x_3 = 0$ ) and the first row of misfit dislocations is given as:  $W_{\text{int}}^{\text{ar1-nw}}(x_0) = \sum_{n=-\infty}^{\infty} W_{\text{int}}^{\text{d-nw}}(x_0 - np)$ , where  $W_{\text{int}}^{\text{d-nw}}(x_0)$  is the energy of the interaction between the nanowire and the misfit dislocation having the line ( $x_1 = 0, x_3 = h$ ).

In order to calculate the energy  $W_{\text{int}}^{\text{d-nw}}$  of the interaction between a nanowire and a dislocation, appearing in formula (1), let us represent the strain field  $\epsilon_{ij}$  created by the nanowire as the sum of the elastic strain  $\epsilon_{ij}$  and the eigenstrain (plastic strain)  $\epsilon_{ij}^*$  which is equal to  $-f_1 \delta_{i1} \delta_{j1} - f_2 \delta_{i2} \delta_{j2}$  inside the nanowire and to zero outside it. Then the energy  $W_{\text{int}}^{\text{d-nw}}$  may be calculated using the general formula [41]:

$$W_{\text{int}}^{\text{d-nw}} = - \int_S \sigma_{ij}^d \epsilon_{ij}^* d\sigma, \quad (7)$$

where  $\sigma_{ij}^d$  is the dislocation stress field, and integration is performed over the area  $S$  of the cross-section of the nanowire. In the case of nanowires with a low angle  $\theta$ , the stress field created

in the nanowire by a dislocation is effectively approximated as the stress field  $\sigma_{ij}^d(x_1, x_3 = 0)$  created by the dislocation on the free surface of the wetting layer when the nanowires are absent. With formulae [41] for the stress field  $\sigma_{ij}^d$  of an edge dislocation near a flat free surface, substituted into formula (7), after integration, we find:

$$W_{\text{int}}^{\text{d-nw}}(x_0) = -\sigma_0 b_1 \tan \theta [g(x_0 + a) + g(x_0 - a) - 2g(x_0)], \quad (8)$$

where

$$g(x) = x \arctan \frac{x}{h} - h \ln(x^2 + h^2). \quad (9)$$

With the formula given in [41], the energy  $W_{\text{int}}^{\text{ar1-f}}$  is calculated as:

$$W_{\text{int}}^{\text{ar1-f}} = -\frac{p_1}{p} \sigma_0 b_1 h_e. \quad (10)$$

Here  $h_e$  is the equivalent thickness of the film, which does not include the thickness of the wetting layer. The thickness  $h_e$  is determined from the condition that the heteroepitaxial layer material has the same volume in the cases of (a) Frank–van der Merwe (continuous) and (b) Stranski–Krastanow growth modes. With this condition, we have  $h_e = a^2 \tan \theta / p_1$ .

By analogy with formula (7) for the energy  $W_{\text{int}}^{\text{d-nw}}$ , in the case  $\theta \ll 1$ , the energies  $W_{\text{int}}^{\text{ar2-nw}}$  and  $W_{\text{int}}^{\text{ar2-f}}$  may be represented in their general forms as follows:

$$\begin{aligned} W_{\text{int}}^{\text{ar2-nw}} &= \varepsilon_{ij}^* S_{\text{nw}} \int_{-\infty}^{\infty} \sigma_{ij}^{\text{ar2}}(x_2, x_3 = 0) dx_2, \\ W_{\text{int}}^{\text{ar2-f}} &= \varepsilon_{ij}^* S_{\text{f}} \int_{-\infty}^{\infty} \sigma_{ij}^{\text{ar2}}(x_2, x_3 = 0) dx_2, \end{aligned} \quad (11)$$

where  $\sigma_{ij}^{\text{ar2}}(x_2, x_3 = 0)$  is the superposition of stress fields created by misfit dislocations belonging to the second row (with dislocation lines perpendicular to nanowires) on the wetting layer free surface when nanowires are absent;  $S_{\text{nw}}$  is the area of the nanowire cross-section, and  $S_{\text{f}}$  the area of a continuous film fragment (characterized by the thickness  $h_e$  and width  $p_1$ ) with the same volume. Since  $S_{\text{nw}} = S_{\text{f}}$ , from formulae (11) one finds  $W_{\text{int}}^{\text{ar2-nw}} = W_{\text{int}}^{\text{ar2-f}}$ .

The surface energy  $\Delta W^{\text{surf}}$  related to the formation of one nanowire (per its unit length) is given as:

$$\Delta W^{\text{surf}} = 2a \left( \frac{\gamma_{\text{lat}}}{\cos \theta} - \gamma_{\text{base}} \right), \quad (12)$$

where  $\gamma_{\text{base}}$  and  $\gamma_{\text{lat}}$  are the specific energies of the wetting layer surface and lateral surfaces of the nanowire, respectively. With formulae (4)–(6), (8)–(10) and (12) substituted into formula (1), and the relation  $W_{\text{int}}^{\text{ar2-nw}} - W_{\text{int}}^{\text{ar2-f}} = 0$ , we find:

$$\begin{aligned} \Delta W^{\text{nw}} &= 2\mu b^2 \left\{ -\frac{2(1+\nu)^2}{\pi(1-\nu)b^2} f_e^2 \tan^2 \theta \left[ 2a^2 \ln 2 + \sum_{n=1}^{\infty} g_2(a, np_1) \right] \right. \\ &\quad \left. - \frac{(1+\nu) \text{sign } b_1 q(x_0, a, p)}{(1-\nu)b} f_e \tan \theta + \frac{a\kappa}{b} \right\}, \end{aligned} \quad (13)$$

where  $b = |b_1|$ ,  $\kappa = [\gamma_{\text{lat}} / \cos \theta - \gamma_{\text{base}}] / (\mu b)$  and

$$q(x_0, a, p) = \sum_{n=-\infty}^{\infty} [g(x_0 - np + a) + g(x_0 - np - a) - 2g(x_0 - np)] - a^2/p. \quad (14)$$

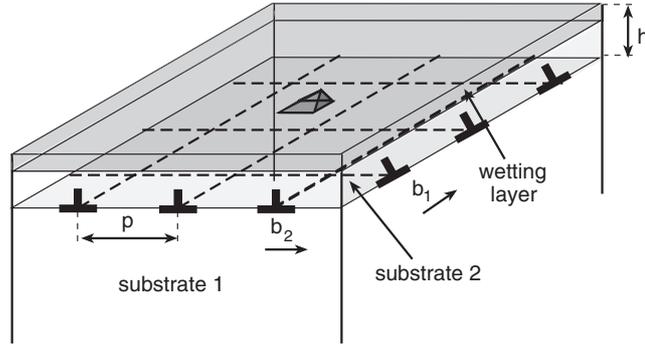


Figure 3. Nano-island (quantum dot) on a composite substrate with misfit dislocations.

#### 4. Quantum dots on dislocated substrates

In this section, we consider the epitaxial growth of quantum dots (three-dimensional growth of nano-islands) on dislocated substrates. For definiteness, as with nanowires (see sections 2 and 3), we assume that quantum dots grow on the wetting layer. The wetting layer is deposited onto a two-layer substrate with misfit dislocations located at the internal interphase boundary between layers 1 and 2 (figure 3). Each quantum dot has the form of a regular pyramid with square base length  $2a$  and small slope angle  $\theta$  formed by the dot lateral facets and the wetting layer plane (figure 3). As with nanowires, quantum dots tend to occupy their equilibrium positions due to the elastic interaction with the misfit dislocations. In our analysis of the growth of quantum dots on the dislocated substrate, we consider the elastically isotropic composite substrate consisting of two layers with the same values of elastic moduli. Also, for definiteness, misfit parameters  $f_1$  and  $f_2$  characterizing the geometric mismatch between crystal lattice parameters of quantum dots and substrate 1 in different crystallographic directions are supposed to be the same:  $f_1 = f_2 = f$ . In these circumstances, as shown in paper [9], the equilibrium positions of quantum dots are located above certain points of the misfit dislocation network consisting of square elementary cells. More precisely, quantum dots tend to occupy the equilibrium positions located above nodes, centre points or diagonal lines of misfit dislocation cells, depending on the misfit dislocation Burgers vectors, misfit  $f$  and values of parameter  $h/p$  [9].

In order to describe the conditions of the energetically favourable formation of quantum dots on the dislocated substrate (figure 3), we calculate the energy difference  $\Delta E^{\text{QD}}$  that characterizes the formation of one quantum dot. In doing so, in fact, we neglect a comparatively low value of the energy that characterizes the elastic interaction between quantum dots.

The energy difference  $\Delta E^{\text{QD}}$  is calculated in a similar way as the energy difference  $\Delta W^{\text{nw}}$  characterizing the formation of nanowires on a dislocated substrate. In our approximation (neglecting the elastic interaction between quantum dots), the energy difference  $\Delta E^{\text{QD}}$  consists of the three basic terms:  $\Delta E^{\text{QD}} = E_{\text{rel}}^{\text{QD}} + \Delta E^{\text{int}} + \Delta E^{\text{surf}}$ . Here  $E_{\text{rel}}^{\text{QD}}$  is the energy of the elastic relaxation of a pyramid-like quantum dot or, in other terms, the difference between the elastic self-energy of the quantum dot and the elastic self-energy of a continuous film fragment with the same volume;  $\Delta E^{\text{int}} = E_{\text{MD-QD}}^{\text{int}} - E_{\text{MD-f}}^{\text{int}}$  is the difference between the energy  $E_{\text{MD-QD}}^{\text{int}}$  that characterizes the interaction of the dislocation rows with the misfit stresses in the quantum dot and the energy  $E_{\text{MD-f}}^{\text{int}}$  that characterizes the interaction of the dislocation rows with the misfit stresses in a continuous film fragment having volume equal to that of one quantum dot, and  $\Delta E^{\text{surf}}$  denotes the surface energy change related to the formation of one quantum dot on

the wetting layer. In our calculations, the energy  $E_{\text{rel}}^{\text{QD}}$  of the elastic relaxation of the pyramid-like quantum dot is approximated by the known expression [37] for the energy of the elastic relaxation that characterizes a quantum dot having conical form. This expression is obtained in the approximation of low value of the slope angle, in which case the Green function for a semi-infinite isotropic medium is used. The approximation in question is good enough in many real situations with quantum dots characterized by low values of the slope angle  $\theta$ .

For illustration, let us consider a quantum dot located above a diagonal line of the misfit dislocation cell and distant by  $x_0$  from the nearest misfit dislocation lines oriented along the axes  $x_1$  and  $x_2$ . In this exemplary case, after some algebra (very similar to that in the previous section dealing with nanowires), we find the following formula for the characteristic energy difference  $\Delta E^{\text{QD}}$ :

$$\Delta E^{\text{QD}} = \frac{1+\nu}{1-\nu} \mu b^3 \left\{ -\frac{8(1+\nu)\psi}{3b^3} a^3 f^2 \tan^2 \theta - \frac{4a^2 \text{sign } b_1}{\pi b^2} \left[ \sum_{n=-\infty}^{\infty} g(x_0 - np) - \frac{4\pi a}{3p} \right] + \frac{4(1-\nu)}{1+\nu} \frac{a^2 \kappa}{b^2} \right\}. \quad (15)$$

Here  $\psi \approx 1.11$ ,  $\kappa = [\gamma_{\text{lat}}/\cos \theta - \gamma_{\text{base}}]/(\mu b)$ , as above and

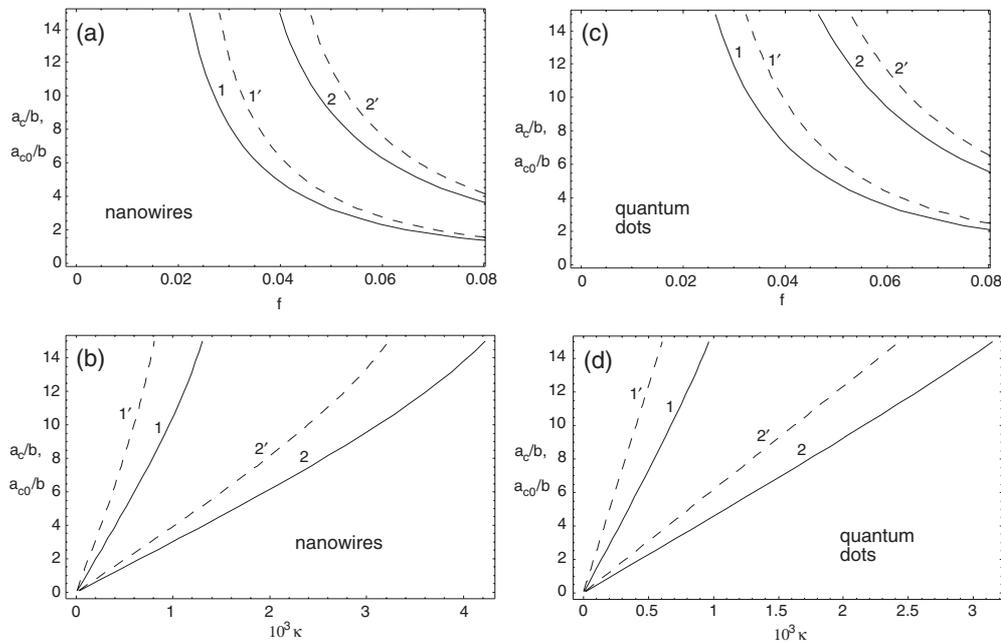
$$g(x) = (a^2 + 3h^2 - x^2) \left( \arctan \frac{a-x}{h} + \arctan \frac{a+x}{h} \right) + 2hx \ln \frac{(a+x)^2 + h^2}{(a-x)^2 + h^2} - 6ah. \quad (16)$$

## 5. Results of models

Thus, we have formulae (13) and (14) for the energy difference  $\Delta W^{\text{nw}}$  that characterizes the formation of nanowires on dislocated substrates (see section 3) as well as formulae (15) and (16) for the energy difference  $\Delta E^{\text{QD}}$  that characterizes the formation of quantum dots on dislocated substrates (see section 4). For simplicity, we will analyse these formulae in the situation where the parameters of the crystal lattice of the epitaxial layer along the axes  $x_1$  and  $x_2$  are the same:  $a_1 = a_2$  and, consequently,  $f_1 = f_2 = f$ . In this situation, the dependences of  $\Delta W^{\text{nw}}$  and  $\Delta E^{\text{QD}}$  on  $a/b$  (not shown in the paper), for characteristic values of parameters (say,  $f = 0.042$ ,  $b_1 = b$ ,  $x_0 = p/2$ ,  $p_1 = p$ ,  $\theta = 11^\circ$ ,  $\nu = 0.3$ ,  $\kappa = 4 \times 10^{-3}$ ,  $h/p = 1/3$ ), have the same character in both the cases with dislocated and non-dislocated substrates. With increasing  $a/b$ ,  $\Delta W^{\text{nw}}$  and  $\Delta E^{\text{QD}}$  first grow and then decrease. It is indicative of the fact that there are critical sizes of nanowires and quantum dots in both the cases discussed, that correspond to maximums of  $\Delta W^{\text{nw}}$  and  $\Delta E^{\text{QD}}$  as functions of  $a/b$ . The growth of a nanowire or quantum dot is energetically favourable if its size is larger than its critical size. In other words, there is some energetic barrier for the formation of nanowires and quantum dots. It is characterized by the critical size of a nanowire or quantum dot, denoted as  $a_c$  and  $a_{c0}$  in the cases with dislocated and non-dislocated substrates, respectively.

The dependencies of  $a_c$  and  $a_{c0}$  for nanowires and quantum dots on parameters  $f$  and  $\kappa$  are shown in figure 4. As follows from figure 4, the presence of misfit dislocations in the substrate is capable of essentially decreasing the critical size of a nanowire or quantum dot (ratio  $a_{c0}/a_c$  may reach 2 for the parameter values used to construct the plots in figure 4). As a corollary, nanowires and quantum dots can grow on dislocated substrates even in the situations where their formation on non-dislocated substrates with the same parameters ( $h$ ,  $f$ ,  $\kappa$ ) is forbidden.

The critical sizes  $a_{c0}$  and  $a_c$  (that characterize the energetically favourable formation of nanowires and quantum dots on non-dislocated and dislocated substrates, respectively) as well as the ratio  $a_{c0}/a_c$  grow with decreasing  $f$  and/or increasing  $\kappa$  (figure 4). This is indicative of the two tendencies. First, the formation of nanowires and quantum dots



**Figure 4.** Dependences of the critical sizes  $a_c$  (solid curves) and  $a_{c0}$  (dashed curves) of nanowires ((a), (b)) and quantum dots ((c), (d)) on misfit parameter  $f$  ((a), (c)) and parameter  $\kappa$  ((b), (d)), for  $p/b = 75$ ,  $\theta = 11^\circ$ ,  $p_1 = p$ ,  $b_1 = b$ ,  $x_0 = p/2$ , and (a), (c)  $h/b = 25$ ;  $\kappa = 1.5 \times 10^{-3}$  (curves 1 and 1') and  $4 \times 10^{-3}$  (curves 2 and 2'); (b), (d)  $h/b = 30$ ;  $f = 0.02$  (curves 1 and 1') and 0.04 (curves 2 and 2').

on a non-dislocated substrate is hampered at low values of misfit  $f$  and shear modulus  $\mu$ , and large values of the specific surface energy  $\gamma_{\text{base}}$  of the wetting layer. This tendency is intuitively evident. Second, with increasing  $\gamma_{\text{base}}$  and/or decreasing  $f$  and  $\mu$ , the effect of misfit dislocations on enhancement of the formation of nanowires and quantum dots becomes more significant (ratio  $a_{c0}/a_c$  increases). To summarize these two tendencies, the misfit-dislocation-induced enhancement of the nucleation of nanowires and quantum dots is well pronounced in heteroepitaxial systems (with large values of  $\gamma_{\text{base}}$  and low values of  $f$  and  $\mu$ ) in which the nucleation of nanowires and quantum dots on non-dislocated substrates is hampered or even energetically forbidden. Large values of  $\gamma_{\text{base}}$  and low values of  $f$  and  $\mu$  are inherent to diverse heteroepitaxial systems which are therefore good candidates for experimental verification of the dislocation-induced enhancement of the nucleation of nanowires and quantum dots.

## 6. Concluding remarks

Thus, in this paper a new mode for the enhanced formation of nanowires and quantum dots—the dislocation-stress-assisted growth of nanowires and quantum dots on composite substrates with misfit dislocations—has been suggested. According to our theoretical analysis, the critical size  $a_c$  that characterizes the energetically favourable formation of nanowires or quantum dots on a dislocated substrate is essentially lower than the critical size  $a_{c0}$  in the case of non-dislocated substrates. This potentially allows one to use the fundamental effects of misfit dislocations on the epitaxial growth in the technologically controlled fabrication and design of semiconductor nanowires and quantum dots with desired functional properties.

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