Perfect, partial, and split dislocations in quantum dots

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A mechanism for relaxation of misfit stresses in nanoislands (quantum dots) is theoretically examined which is the formation of partial and split misfit dislocations. The parameters of nanoislands with perfect, partial, and split misfit dislocations are estimated and compared, with emphasis on the case of Ge/Si nanoislands. Different dislocation structures are shown to be energetically preferred in different regions of the nanoisland/substrate interface. It is theoretically revealed that perfect misfit dislocations (conventionally considered in models of dislocated nanoislands) are not energetically favorable in pyramidlike nanoislands in Ge/Si system. Also, it is shown that misfit dislocation formation is capable of causing nanoisland shape transformation as an energetically favorable process.

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I. INTRODUCTION

Self-assembled semiconductor nanoislands (quantum dots) exhibit unique functional properties, being the subject of intensive fundamental research and opening up a range of new applications; see, e.g., Refs. 1–15. Of special interest are applications of semiconductor nanoislands in novel electronic and optoelectronic devices with reduced size and weight. The structure and geometric shape of nanoislands are among the most important issues for these applications. In particular, the formation of misfit dislocations in nanoislands and transformations of their shape can cause serious performance problems for semiconductor nanodevices. In this context, identification of conditions, at which these processes occur in semiconductor nanoislands, is of utmost significance. It is a serious problem for experimental analysis, because of extremely high demands for precise measurements at nanoscale. In these circumstances, theoretical models of structural and shape transformations of semiconductor nanoislands are very important for understanding the fundamentals of nanoscale effects in semiconductors as well as for fabrication and design of electronic nanodevices with stable functional characteristics.

Current theoretical models of dislocations in strained nanoislands conventionally deal with perfect misfit dislocations [Fig. 1(a)]; see, e.g., Refs. 1,13–15. Recently, a physical mechanism for stress relaxation in nanoislands has been suggested which is the formation of partial and split dislocations [Figs. 1(b) and 1(c)].[16] Perfect misfit dislocations [Fig. 1(a)] violate the coherency of the nanoisland/substrate boundary only at line dislocation cores. The formation of two partial dislocations composing a split configuration [Fig. 1(b)] or a single partial dislocation [Fig. 1(c)] is accompanied by formation of a stacking fault, in which case the ideal coherency of the nanoisland/substrate boundary is violated at both local dislocation cores and extended stacking fault plane. In addition, stress field distributions created by perfect, partial and split dislocations are different. Therefore, nanoislands with perfect [Fig. 1(a)], split [Fig. 1(b)], and partial [Fig. 1(c)] misfit dislocations have different characteristics sensitive to the nanoisland/substrate boundary structure and stress field distribution in the nanoisland. Also, the formation of perfect, split and partial dislocations in a nanoisland becomes energetically favorable at different critical values of its geometric and material parameters, in which case it is important to identify the most favorable type of misfit dislocations (whose formation leads to dramatic degradation of functional characteristics of quantum dots). The aforesaid causes high interest to a detailed theoretical description of the competition between the standard [Fig. 1(a)] and the earlier briefly considered[16] relaxation mechanisms in strained nanoislands. The main aim of this paper is to theoretically examine in detail the competition in question, with focuses placed on the conditions at which the generation of split and partial misfit dislocations [Figs. 1(b) and 1(c), respectively] in a strained nanoisland is energetically favourable. Also, we will theoretically examine the effect of misfit dislocation formation on nanoisland shape transformations.

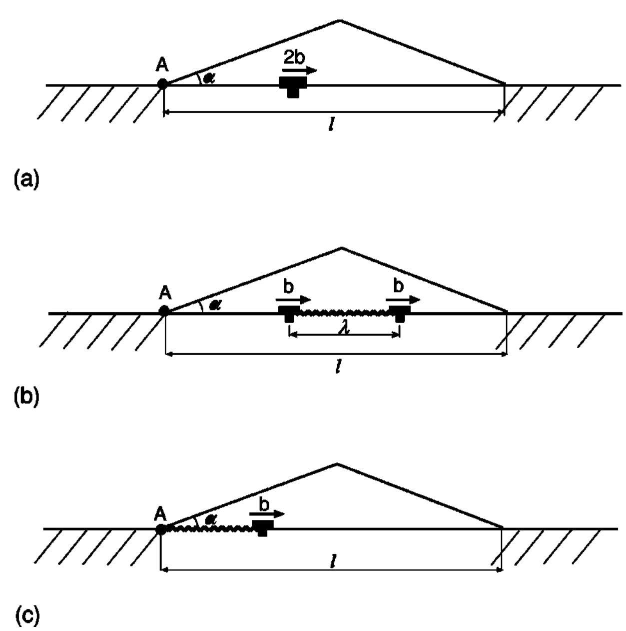

FIG. 1. Misfit dislocation configurations in pyramidlike nanoisland (quantum dot): (a) Perfect misfit dislocation, (b) two partial misfit dislocations joined by stacking fault, and (c) one partial misfit dislocation joined by stacking fault with a lateral node point.

II. PERFECT MISFIT DISLOCATIONS IN NANOISLANDS: SHAPE TRANSFORMATIONS OF DISLOCATED NANOISLANDS

Let us consider a model heteroepitaxial system consisting of a nanoisland and a semi-infinite substrate (Fig. 1). The nanoisland has the form of a regular pyramid with the rectangular base edge length l and the slope angle α formed by the island lateral facets and the substrate plane. The nanoisland and the substrate are assumed to be elastically isotropic materials with the same values of the shear strength G and the same values of the Poisson ratio ν. Misfit stresses occur in the nanoisland due to the misfit (geometric mismatch) between the crystal lattice parameters a_i and a_s of the island and the substrate, respectively. For simplicity, here and in the following we confine our consideration to the two-dimensional model system (Fig. 1) with one-dimensional misfit $f=2(a_s-a_i)/(a_s+a_i)$.

Now let us consider the generation of a perfect misfit dislocation at the lateral node point A (where the lateral facet of the nanoisland connects the substrate free surface) and its consequent motion along the nanoisland/substrate interface towards the island base center (Fig. 1). The generation of the misfit dislocation is energetically favourable, if the energy difference $\Delta W=W-W^f<0$, where W^f and W are the energies of the nanoisland in the coherent (dislocation-free) state and the dislocated state (Fig. 1), respectively. The exact analytical calculation of the energy of the dislocated nanoisland on the substrate needs exact analytical formulas for the stress field and elastic energy of an edge dislocation located near the curved free surface formed by the free surfaces of the nanoisland and the substrate (Fig. 1). Up to now, however, as to the authors knowledge, such formulas have not been derived. In these circumstances, in calculations of this paper, instead of unknown formulas for stress fields of dislocations near curved free surface, we will use in the first approximation the analytical formulas[17] for stress fields of a straight dislocation near a cylindrical solid. To do so, we will model the nanoisland/substrate system as a cylindrical composite solid of radius R and infinite length (Fig. 2). The interphase nanoisland/substrate boundary represents a strip which is parallel with the cylinder center axis and makes an angle α with the cylinder free surface (Fig. 2). In the coordinate system shown in Fig. 2, the interphase boundary occupies the region ($|x|<l/2=R\sin\alpha, y=y_0=R\cos\alpha$), and the misfit dislocation is located at $(x=x_0, y=y_0)$ and has the Burgers vector $2\boldsymbol{b}=2b\boldsymbol{e}_x$.

The model (Fig. 2) in question is effective in the case of low angles α, where the form of the nanoisland/substrate composite is close to that of the cylinder. In particular, it is the case of Ge/Si (100) nanoislands (with $\alpha=11°$) that have a great technological potential. However, even for small α, the suggested model is weakly effective in a description of a misfit dislocation located in the vicinity of the lateral point A, where the straight free surface of the substrate and a straight nanoisland facet that make a contact angle α are modeled as the continuously curved free surface of cylinder. It is the general weak point of models of dislocation generation in nanoislands and solid films, using methods of the elasticity theory; see, e.g., Refs. 13–21. Such models commonly do not describe in a strict manner the behavior of a dislocation near a free surface point of its entering into a film or nanoisland, because it needs a detailed description of such "hidden" factors as the atomic arrangements at the dislocation core and the free surface. At the same time, details of the behavior of a dislocation near the free surface point of its entering into a film or nanoisland are not essential for understanding the conditions at which the dislocation formation in the film or nanoisland is energetically favorable. The fact is that a dislocation is able to overcome a barrier in the region considered due to thermal fluctuations that facilitate motion of double kinks of dislocation line. In these circumstances, the knowledge of energetic characteristics of a dislocation distant from the nanoisland free surface allows one to understand, if the dislocation generation (crucially affecting the functional properties of quantum dots) in the nanoisland is favorable. The suggested model (Fig. 2) is effective in a description of dislocations distant from the nanoisland free surface, in which case we think conclusions based on its results (see next sections) to be reasonable enough.

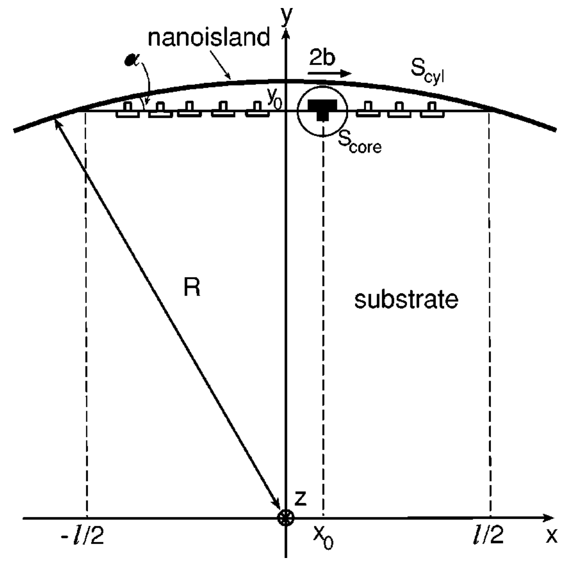

FIG. 2. Perfect misfit dislocation in two-phase cylinder. Misfit between crystal lattice parameters of the nanoisland and the substrate is modeled as that associated with a continuous distribution of virtual misfit dislocations at the interphase boundary.

In the framework of the model considered, the elastic energy of the nanoisland containing a perfect misfit dislocation consists of the four terms

$$W=W^f+W^d(x_0,2b)+W^{d-f}(x_0,2b)+W^c(2b). \quad (1)$$

Here W^f denotes the misfit strain energy, $W^d(x',b')$ the proper elastic energy of the perfect misfit dislocation (with Burgers vector $b'\boldsymbol{e}_x$) located at $x=x'$, $W^{d-f}(x',b')$ the elastic energy associated with the elastic interaction between the dislocation and the misfit stresses, and $W^c(2b)$ the energy of the dislocation core. The generation of the perfect dislocation is energetically favorable, if it leads to a decrease of the total energy, that is, if $\Delta W=W-W^f<0$. With formula

(1) taken into account, we come to the following criterion for the generation of the perfect misfit dislocation to be energetically favorable:

$$\Delta W = W^d(x_0,2b) + W^{d-f}(x_0,2b) + W^c(2b) < 0. \quad (2)$$

Let us calculate the terms appearing on the right hand side of formula (2). The dislocation core energy is conventionally[22] written as $W^c(b') \approx Db'^2/2$, where $D = G/[2\pi(1-\nu)]$. Following Ref. 22, the proper elastic energy of the dislocation is given by the formula

$$W^d(x',b') = \frac{Db'^2}{2}\left(\left.\frac{\partial\chi}{\partial y}\right|_{S_{\rm core}} - \left.\frac{\partial\chi}{\partial y}\right|_{S_{\rm cyl}}\right). \quad (3)$$

Here $S_{\rm cyl}$ denotes the model cylinder free surface, $S_{\rm core}$ the surface of cylinderlike dislocation core of radius b, and χ the stress function for the dislocation in cylinder,[23] which may be presented in the form[24]

$$\chi(x,y) = \frac{Db'}{2}\left((y-y_0)\ln\frac{C^2r^2}{P^2R^2} + \frac{y_0(r^2-R^2)(x'^2+y_0^2-R^2)}{R^2C^2} + \frac{yR^2P^2}{r^2C^2}\right), \quad (4)$$

where $P^2 = (x'-x)^2 + (y_0-y)^2$, $C^2 = (x'-xR^2/r^2)^2 + (y_0 - yR^2/r^2)^2$, and $r^2 = x^2 + y^2$.

It should be noted that formula (3) is approximate. Derivative $\partial\chi/\partial y$ appearing in this formula is constant on the cylinder free surface $S_{\rm cyl}$ (due to zero-traction conditions at the surface), but is different in different points of the dislocation core surface $S_{\rm core}$. In order to decrease a calculation error related to the difference between values of $\partial\chi/\partial y$ in different points of the dislocation core (this difference is essential, if the distance between the dislocation core and the cylinder free surface is of the same order as b'), we represent $(\partial\chi/\partial y)|_{S_{\rm core}}$ as the mean value of $\partial\chi/\partial y$ taken in the two opposite points of the dislocation core

$$\left.\frac{\partial\chi}{\partial y}\right|_{S_{\rm core}} = \frac{1}{2}\left(\frac{\partial\chi}{\partial y}(x'-b',y_0) + \frac{\partial\chi}{\partial y}(x'+b',y_0)\right). \quad (5)$$

With Eqs. (4) and (5) substituted into formula (3), we get $W^d(x',b') = (Db'^2/4)G(\tilde{x}',\tilde{y}_0,\tilde{r}_0)$, where

$$G(\tilde{x}',\tilde{y}_0,\tilde{r}_0) = (M_+ - 1)[1 - 2\tilde{y}_0^2(M_+ + 1)] + (M_- - 1)\times[1 - 2\tilde{y}_0^2(M_- + 1)] - \ln(M_+M_-), \quad (6)$$

$$M_\pm = \frac{\tilde{r}_0^2}{\tilde{y}_0^4 + (\tilde{x}'^2 + (\tilde{x}' \pm \tilde{r}_0)^2 - 2)\tilde{y}_0^2 + (\tilde{x}'^2 \pm \tilde{r}_0\tilde{x}' - 1)^2}, \quad (7)$$

$\tilde{x}' = 2\sin\alpha x'/l$, $\tilde{y}_0 = 2\sin\alpha y_0/l$, and $\tilde{r}_0 = 2\sin\alpha b'/l$.

Now let us turn to analysis of term $W^{d-f}(x',b')$ appearing in formula (2). It is calculated as the energy that characterizes the elastic interaction of the perfect misfit dislocation with continuously distributed virtual dislocations (modeling misfit) at the interphase boundary (Fig. 2):

$$W^{d-f}(x',b') = \int_{-l/2}^{l/2}\frac{dW^{d-d}(x',x,b')}{dx}dx. \quad (8)$$

Here $dW^{d-d}(x',x,b')$ is the energy of the interaction between the perfect misfit dislocation [located at (x',y_0)] with Burgers vector $\boldsymbol{b}'$ and a virtual dislocation [located at (x,y_0)] with infinitesimal Burgers vector $d\boldsymbol{b} = -f dx \boldsymbol{e}_x$. The energy dW^{d-d} is calculated using the formula[23]

$$dW^{d-d}(x',x,b') = -Db'f dx\left(\frac{\partial\chi}{\partial y}(x,y_0) - \left.\frac{\partial\chi}{\partial y}\right|_{S_{\rm cyl}}\right). \quad (9)$$

With Eqs. (4) and (9) substituted into Eq. (8), we find $W^{d-f}(x',b') = -Dlb'fH(\alpha,\tilde{x}')$, where

$$H(\alpha,\tilde{x}') = \frac{\sin^2\alpha - \tilde{x}'^2}{\sin\alpha(\cos^2\alpha - \tilde{x}'^2)^3}\Big\{-2\sin\alpha(\cos^2\alpha + \tilde{x}'^2)\times(\sin^4\alpha - (\tilde{x}'^2+3)\sin^2\alpha + 2) - (2\alpha - \pi)\cos\alpha(\sin^4\alpha - (2\tilde{x}'^2+3)\sin^2\alpha + \tilde{x}'^4 - \tilde{x}'^2 + 2) + \tilde{x}'(\sin^4\alpha - (2\tilde{x}'^2+5)\sin^2\alpha + \tilde{x}'^4 + \tilde{x}'^2 + 4)\ln\frac{\sin\alpha + \tilde{x}'}{\sin\alpha - \tilde{x}'}\Big\}. \quad (10)$$

From formulas (2), (6), (7), (10), with $W^c(b') = Db'^2/2$, we have the following expression for the energy difference ΔW related to the formation of the perfect misfit dislocation in a nanoisland [Fig. 1(a)]:

$$\Delta W = \frac{Db'^2}{4}\left.\left(G(\tilde{x}',\tilde{y}_0,\tilde{r}_0) - \frac{4lf}{b'}H(\alpha,\tilde{x}') + 2\right)\right|_{b'=2b,x'=x_0}. \quad (11)$$

Dependence of ΔW on the coordinate x_0 of a perfect misfit dislocation is shown in Fig. 3, for various values of misfit parameter f. As it follows from Fig. 3, there is an energetic barrier ($\Delta W > 0$) for generation of the perfect misfit dislocation near lateral facets of the nanoisland. At the same time, the presence of the perfect misfit dislocation in a central area of the interphase (island/substrate) boundary is energetically favorable ($\Delta W < 0$). It is similar to the conventional situation[20] with thermal-fluctuation-assisted generation of a misfit dislocation at the continuous film free surface (where the dislocation is not energetically preferred) and its motion to the film/substrate boundary (where the dislocation is preferred).

Let us reveal the ranges of parameters at which the existence of the perfect misfit dislocation at the nanoisland base center ($x_0 = 0$) is energetically favorable compared to the coherent state of the interphase boundary. The necessary criterion ($\Delta W < 0$) for the dislocation existence to be favorable can be rewritten, with Eq. (11), in the form $f > f_c$, where the critical misfit parameter is given as

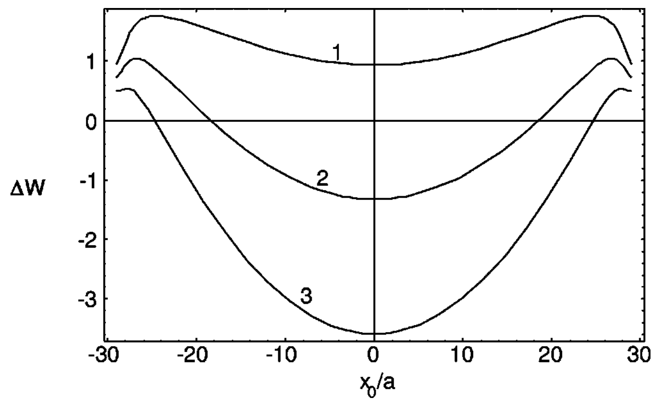

FIG. 3. Dependences of the energy difference ΔW (in units of $Da^2/2$), related to the dislocation formation in Ge/Si(100) nanoisland, on dislocation configuration coordinate x_0/a (see text), for $\alpha=11°$, $l=60b$, and $f=0.04$, 0.06, and 0.08 (see curves 1, 2, and 3, respectively) .

$$f_c=\frac{b'[G(\tilde{x}',\tilde{y}_0,\tilde{r}_0)+2]}{4lH}\bigg|_{x'=0,b'=2b}. \qquad (12)$$

Dependence of the critical misfit f_c on the characteristic angle α, given by formula (12), is shown in Fig. 4, for the various values of the nanoisland base length l. From Fig. 4 it follows that f_c decreases with rising the base length l at given angle α. Also, f_c has minimum in the range of $\alpha=38.1°\pm0.5°$, for l having a constant value in the range from $30a$ to $300a$. This allows us to conclude that a nanoisland with a given base length l has the critical angle α_c at which the formation of the perfect misfit dislocation is most favorable. Dependences of $\Delta W|_{x=x_0}$ on angle α [which are calculated using formula (12) and, for simplicity, are not presented in this paper], for various values of l, also have minimums at $\alpha\approx38°$ in wide ranges of l and f. Thus, the perfect misfit dislocation formation is most favourable in nanoislands with the same base length, if their characteristic angle $\alpha\approx38°$.

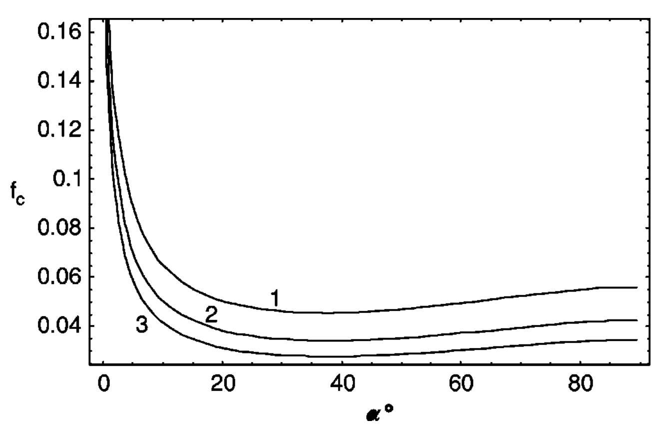

FIG. 4. Dependences of critical misfit parameter f_c (that characterizes energetically favorable generation of a perfect misfit dislocation at nanoisland base center) on nanoisland slope angle α, for $l/a=40$, 60, and 80 (curves 1, 2, and 3, respectively).

It should be noted that $\alpha=38°$ is not a low angle. It causes a question about validity of the model representation of a nanoisland/substrate system as a composite cylinder (with small upper part and large bottom part of cylinder representing the nanoisland and the substrate, respectively, see Fig. 2). In our previous analysis of energetic characteristics of a misfit dislocation located in arbitrary position at the nanoisland/substrate interface, the model is effective at only low values of slope angle α. However, if the misfit dislocation is located at the nanoisland base center, the model can be effectively applied to the case of intermediate values of α, too. More presicely, with the key role of free surfaces as that causing the screening effect on dislocation stress fields, our model (Fig. 2) is effective when it correctly takes into account the screening effect. Following the analysis of dislocation stress fields near free surfaces,[25] the screening length of the stress fields induced by a dislocation is the double distance between the dislocation and the nearest free surface. This allows us to think that our model (Fig. 2) is effective in description of a misfit dislocation at the nanoisland base center when the distance between the dislocation and the model nanoisland free surface is lower by at least a factor of 2, compared to the distance between the dislocation and the model substrate free surface. It corresponds to range of $\alpha\leqslant53°$.

Now let us consider potential changes of the shape of a nanoisland, associated with the formation of a perfect misfit dislocation. In doing so, we will find the angle α characterizing the nanoisland shape at given value of the nanoisland volume, that minimizes the energy difference ΔW. In the framework of our model, a nanoisland represents a fragment of infinite cylinder, having a constant area S of the section perpendicular to the interphase boundary (Fig. 2). This area is in the following relationship with the nanoisland base length l and slope angle α, $S=l^2(2\alpha-\sin 2\alpha)/[4(1-\cos 2\alpha)]$, which can be rewritten as

$$l=\sqrt{4S(1-\cos 2\alpha)/2\alpha-\sin 2\alpha}. \qquad (13)$$

With Eq. (13) substituted into Eq. (11), we represent ΔW as a function of parameters f, α, and S.

Dependences of $\Delta W|_{x_0=0}$ on α are shown in Fig. 5, for various values of S and f. As follows from Fig. 5, minimums of ΔW (at given constant value of S) correspond to angle $\alpha=\alpha_m\approx19°$. [More precisely, for $f=0.04-0.1$ and $l(\alpha_m)=(40-180)a$, minimums of ΔW correspond to $\alpha=\alpha_m=19°\pm2°$.] The aforesaid, in the framework of our model, indicates that the misfit dislocation formation in a nanoisland is capable of causing its shape transformation driven by a release of the nanoisland energy. This conclusion is supported by data of paper[9] reporting experimental observation of nanoisland shape transformations that accompany the misfit dislocation formation.

In Fig. 5, the angle α_m giving minimum ΔW is almost the same ($\alpha_m\approx19°$) regardless of various values of parameters S and f. It can be attributed to the crucial influence of the angular, θ dependence of the dislocation stress field on transformations of nanoisland shape, where θ is the angle coordi-

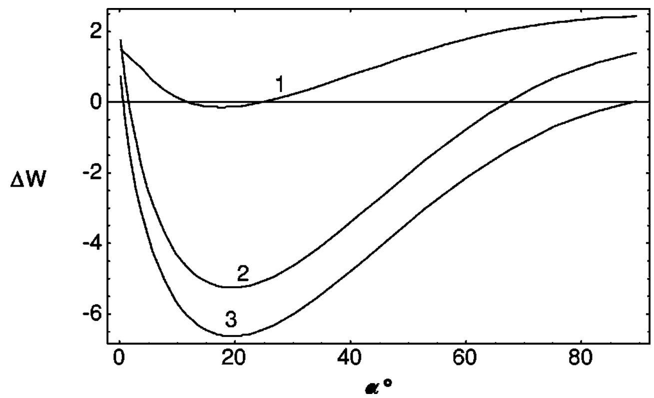

FIG. 5. Dependences of the energy difference ΔW (in units of $Da^2/2$), related to the misfit dislocation formation at nanoisland base center, on nanoisland slope angle α, for the following combinations of parameters: ($f=0.04$, $S=200a^2$), ($f=0.04$, $S=800a^2$), ($f=0.08$, $S=200a^2$) (see curves 1, 2, and 3, respectively).

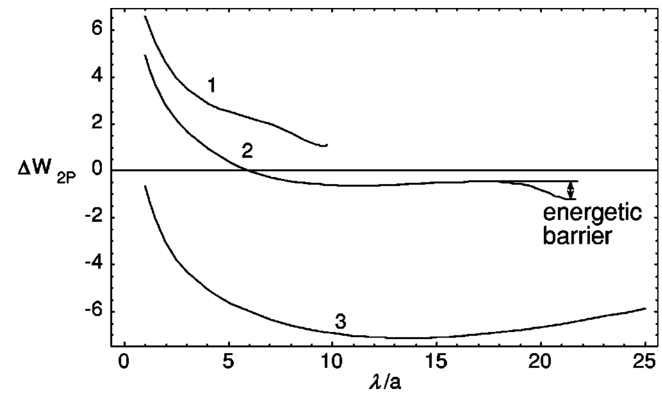

FIG. 6. Dependences of the energy difference ΔW_{2P} (in units of $Da^2/2$), related to the formation of two partial misfit dislocations, on λ/a, for $x_0/a=45$, 39 and 25 (curves 1, 2, and 3, respectively).

nate in the cylindrical coordinate system associated with the dislocation line. Actually, this dependence is insensitive to misfit parameter f and nanoisland base length l. At the same time, a dislocation creates stresses whose spatial distribution is different in nanoislands with different shapes due to the namely angular dependence in question. In the context discussed, shape transformations of dislocated nanoislands are expected to be strongly affected by such characteristics of misfit dislocation as its Burgers vector orientation and spatial position at the interface, which determine the angular dependence of the dislocation stress field within a nanoisland.

III. PARTIAL AND SPLIT DISLOCATION STRUCTURES IN QUANTUM DOTS (NANOISLANDS)

In the previous section, we have theoretically considered perfect misfit dislocations formed in nanoislands. In general, as with continuous films,[26,27] partial and split misfit dislocations can be generated in nanoislands. In Ref. 16 in the first approximation it has been demonstrated that split misfit dislocations can be more energetically favorable than perfect dislocations in nanoislands. In this section, in the framework of our approach (see Sec. II) which is more detailed than the first approximation model,[16] we will examine in detail conditions at which the split and partial misfit dislocations are preferred in nanoislands.

Let us consider a nanoisland containing (a) two partial misfit dislocations with a stacking fault between them [Fig. 1(b)] or (b) one partial misfit dislocation with a stacking fault between it and lateral node point A [Fig. 1(c)], the starting point of the dislocation motion. To characterize these dislocation configurations, we will calculate the energy difference ΔW_{1P} and ΔW_{2P} related to the formation of one [Fig. 1(c)] and two [Fig. 1(b)] partial misfit dislocations in the nanoisland with initially coherent interphase boundary. Then, in order to distinguish the most favourable dislocation configuration from those shown in Fig. 1, we will compare their energetic characteristics ΔW, ΔW_{1P}, and ΔW_{2P}.

The energy difference ΔW_{2P} can be written as follows:

$$\Delta W_{2P}=W^d(x_1,b)+W^d(x_2,b)+W^{d-f}(x_1,b)+W^{d-f}(x_2,b)+2W^c(b)+W^{1-2}+W^{\gamma}. \quad (14)$$

Here W^{1-2} denotes the energy that characterizes the elastic interaction between the partial misfit dislocations, W^{γ} is the stacking fault energy, x_1 and x_2 are the coordinates of the first and second dislocations, respectively, which are in the following relationships with the interspacing λ between the dislocations and x_0 playing the role of the stacking fault center: $x_1=x_0-\lambda/2$, $x_2=x_0+\lambda/2$. The energies W^d and W^{d-f} appearing on the right hand side of formula (14) are given by formulas (6), (7), and (10), respectively. $W^c(b')=Db'^2/2$.[22] The energy W^{1-2} is calculated using formula $W^{1-2}=dW^{d-d}(x_1,x_2,b)/dx|_{f=-b}$, with dW^{d-d} given by formulas (4) and (9). The energy W^{γ} is conventionally as follows: $W^{\gamma}=\gamma(x_2-x_1)$, where γ denotes the specific energy (per unit area) of the stacking fault.

Dependences of ΔW_{2P} on λ/a, given by formula (14), are shown in Fig. 6 in the case of Ge/Si nanoislands characterized by the following values of parameters[28] $f=0.042$, $a=0.566$ nm, $\gamma=6.9\times10^{-2}$ J/m^2, $G=40$ GPa, $\nu=0.26$, and $x_0/a=45$, 39, and 25 (see curves 1, 2, and 3, respectively). The left end point of each curve in Fig. 6 corresponds to the limiting situation where the partial dislocations [Fig. 1(b)] are distant from each other by minimum interspacing a. The right end point of each curve in Fig. 6 corresponds to enter of the second partial dislocation into the nanoisland.

When the first partial dislocation is close to a lateral node point (see curve 1 that corresponds to large $|x_0|$), the characteristic energy difference $\Delta W_{2P}(\lambda)$ is always positive. That is, the generation of the second partial dislocation is energetically unfavorable.

When the first partial dislocation moves towards the nanoisland base center ($|x_0|$ decreases), character of dependence $\Delta W_{2P}(\lambda)$ changes; see curve 2 in Fig. 6. More precisely, $\Delta W_{2P}(\lambda)$ is negative in some range of λ, and there is a point $\lambda=\lambda_0$ where $\Delta W_{2P}(\lambda)$ takes a minimum. As a corollary, the existence of the two partial misfit dislocations [Fig. 1(b)] joined by the stacking fault is energetically favorable in the nanoisland. It is most favorable, if stacking fault size is λ_0. However, ΔW_{2P} increases when λ changes from

$22a$ (it corresponds to enter of the second dislocation into the nanoisland) to $18a$; see curve 2 in Fig. 6. Therefore, the generation and consequent movement of the second partial dislocation towards its equilibrium position (where the two-dislocation configuration [Fig. 1(b)] is characterized by the minimum energy) need an energetic barrier to be overcome.

[Generally speaking, the second minimum of $\Delta W_{2P}(\lambda)$ at $\lambda = 21a$ may be distingiushed at curve 2 in Fig. 6. However, it corresponds to the situation where the second dislocation is distant by a from the lateral node point. At the same time, quantitative predictions of our model are not exact in this situation; see discussion in Sec. II. Therefore, in our analysis we do not take into consideration the minimum at $\lambda = 21a$.]

When the first partial dislocation is close to the nanoisland base center (see curve 3 in Fig. 6), the energetic barrier for the formation of the two-dislocation configuration [Fig. 1(b)] disappears. Actually, with decreasing λ from $25a$ (it corresponds to enter of the second dislocation into the nanoisland) to $13a$ [where $\Delta W_{2P}(\lambda)$ takes its minimum], the characteristic energy difference ΔW_{2P} gradually decreases. That is, the generation and consequent movement of the second misfit dislocation to its equilibrium position where ΔW_{2P} is minimum occur in a nonbarrier way.

Now let us consider the energy difference ΔW_{1P} characterizing the formation of one partial misfit dislocation [Fig. 1(c)] in a nanoisland with initially coherent interphase boundary. According to the calculation scheme used in this paper, the energy difference in question can be written as follows:

$$\Delta W_{1P} = W^d(x_0, b) + W^{d-f}(x_0, b) + W^c(b) + \widetilde{W}^\gamma. \quad (15)$$

Here $\widetilde{W}^\gamma = \gamma(l/2 + x_0)$ is the stacking fault energy, and x_0 denotes the coordinate of the partial misfit dislocation.

Comparison of the characteristic energies ΔW_{2P}, ΔW_{1P}, and ΔW allows one to reveal the most energetically favorable structure of the interphase boundary and its transformations, depending on parameters of the nanoisland. We have calculated with the help of the above formulas the dependences of $\Delta W_{2P}|_{\lambda=\lambda_0}$, ΔW_{1P}, and ΔW on x_0, where x_0 plays the role of the coordinate of respectively the perfect MD and the partial MD in the cases shown in Figs. 1(a) and 1(c), respectively; and x_0 is the coordinate of the stacking fault center in the case of two partial MDs [Fig. 1(b)]. (In calculation of dependences of $\Delta W_{2P}|_{\lambda=\lambda_0}$ on x_0, we have used as an input the analytical functions (exhibited as curves 4 in Fig. 7) being interpolations of numerically calculated dependences $\lambda_0(x_0)$ (dashed curves in Fig. 7). In doing so, $\lambda_0(x_0)$ is the interspacing between the two partial misfit dislocations [Fig. 1(b)], that corresponds to minimum value of ΔW_{2P}.) The calculated dependences are presented in Fig. 7, for various values of characteristic parameters l and α of nanoislands. For given value of x_0, the lowest dependence from the set ($\Delta W_{2P}|_{\lambda=\lambda_0}$, ΔW_{1P}, ΔW) of dependences shown in Fig. 7 specifies the most energetically favorable misfit dislocation configuration at this value of x_0.

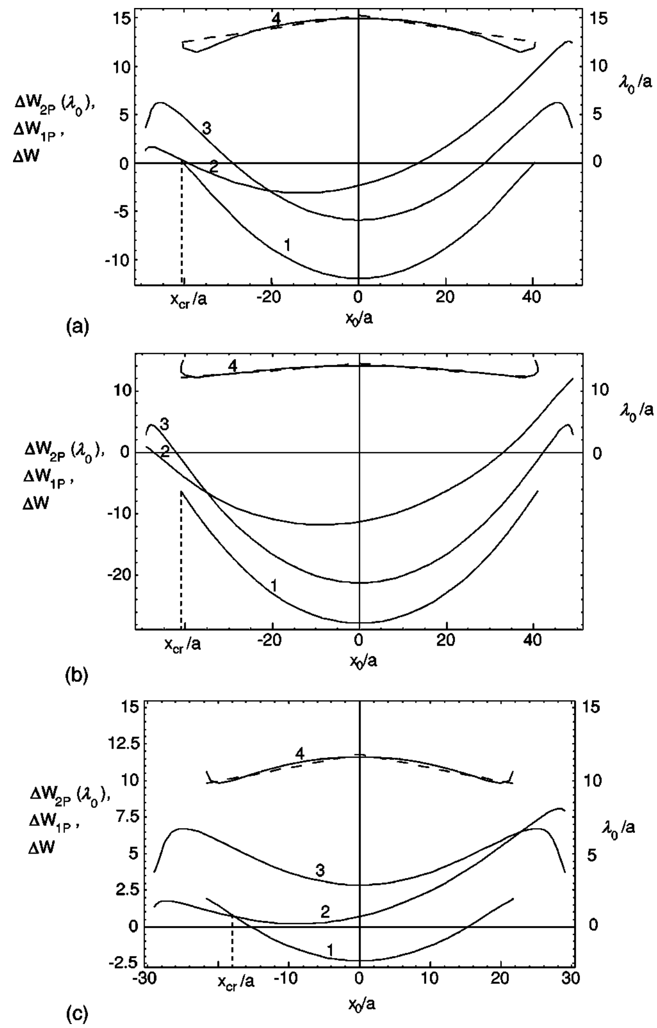

FIG. 7. Dependences of the energetic characteristics (in units of $Da^2/2$), ΔW_{2P} (curve 1), ΔW_{1P} (curve 2), and ΔW_{L-C} (curve 3), of Ge/Si nanoisland on dislocation configuration coordinate x_0/a (see text). Numerically calculated dependences $\lambda_0(z)$ are shown as dashed curves. Their analytical interpolations are shown as solid curves 4. (a), (b), and (c) correspond to cases with $l = 100a$, $\alpha = 11°$; $l = 100a$, $\alpha = 25°$; and $l = 60a$, $\alpha = 11°$, respectively.

As follows from Fig. 7, a single partial dislocation [Fig. 1(c)] is the most favorable dislocation configuration in vicinity of a lateral node point of the nanoisland, since the energy ΔW_{1P} (curve 2) in this region is lowest among the energies characterizing the dislocated states of a nanoisland. However, ΔW_{1P} is negative in the vicinity of a lateral node point in only the situation shown in Fig. 7(b), indicating that the dislocation generation occurs in a nonbarrier way. ΔW_{1P} that characterizes a single partial dislocation near the lateral node point is positive in the situations shown in Figs. 7(a) and 7(c). It means that the coherent (nondefect) state is preferred, while the dislocation generation needs an energetic barrier to overcome. In general, when the single partial dislocation is generated, its movement towards the nanoisland base center is driven by a release of the nanoisland energy. It is indicated as a decrease of ΔW_{1P} with decreasing $|x_0|$ that characterizes spatial position of the single partial dislocation. For $|x_0|$

exceeding some critical value $|x_{cr}|$ dependent on parameters of the nanoisland, curve 1 (which depicts the energy change ΔW_{2P} due to the formation of two partial dislocations [Fig. 1(b)]), becomes the lowest one among curves characterizing the dislocated states of the nanoisland. More than that, it is negative at almost any $|x_0|$. In the parameter region discussed, a pair of partial dislocations [Fig. 1(b)] is most favorable. As it follows from Fig. 7(a), perfect misfit dislocation [Fig. 1(a)] is not favorable at any $|x_0|$ (see curve 3).

Thus, a single partial dislocation [Fig. 1(c)] is the most energetically favorable dislocation configuration in vicinity of a lateral node point of the nanoisland. During movement of the partial dislocation towards the nanoisland base center, which is driven by a release of the nanoisland energy, the generation of the second partial dislocation [Fig. 1(b)] becomes energetically favorable. The transformation of the state with one partial dislocation [Fig. 1(c)] into the state with two partial dislocations [Fig. 1(b)] occurs as an energetically favorable process when the coordinate x_0 of the first partial dislocation reaches its critical value x_{cr} sensitive to parameters of the nanoisland.

Notice that the model used in this paper is too approximate to make strict conclusions on the dislocation type if it is located near an island free surface (see discussion in Sec. II). In any event, however, results of our analysis indicate that partial [Fig. 1(c)] and split misfit dislocation [Fig. 1(b)] structures are energetically favorable in nanoislands in wide ranges of their parameters.

Our conclusions on the dislocated structure of nanoislands, based on the analysis of their equilibrium energetic characteristics, describe the nanoislands at quasiequilibrium conditions. However, nanoislands are commonly formed at highly nonequilibrium conditions, in which case kinetic factors come into play. This can cause some disagreement between our theoretical estimates and experimental data. In any case, however, the stress relaxation via formation of partial and split misfit dislocation configurations in strained nanoislands should be definitely taken into account in future experimental and theoretical studies of nanoislands. In particular, distribution of stresses created by partial and split misfit dislocation configurations is more spatially homogeneous, compared to that created by a perfect misfit dislocation. As a corollary, stress-assisted processes (diffusion, island shape transformations, formation of trenches near the islands, rearrangements of nanoisland ensembles, etc.) which influence the functional properties of nanoislands occur in different ways in the case with partial misfit dislocations and the conventionally modeled case with a perfect misfit dislocation.

IV. CONCLUDING REMARKS

Thus, in this paper, we have theoretically examined in detail the earlier briefly discussed[16] relaxation mechanism in strained nanoislands, namely, the generation of split and partial misfit dislocation configurations [Figs. 1(b) and 1(c)]. According to our theoretical analysis, the generation of partial and split misfit dislocations are energetically favorable compared to conventional perfect misfit dislocations in wide ranges of structural and geometric characteristics of pyramidlike nanoislands in the Ge/Si system. In this context, degradation of functional properties of quantum dots, associated with dislocation generation, should be experimentally examined and theoretically described in the future, with the behavioral features of the partial and split dislocations taken into account. Of special importance will be experimental identification of the misfit dislocation type (perfect, partial, or split) in strained nanoislands with various compositions and geometric parameters. This potentially allows one to use technologically controlled parameters (misfit parameter, crystallography of interphase boundary, etc.) of nanoislands in fabrication and design of such islands with desired structure and properties. The results of the approximate analysis of this paper can be used also in studies of the influence of free surfaces on partial dislocation structures that often exist in quasicrystals,[29,30] bulk semiconductors,[31,32] and superconductors.[33,34]

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