Relaxation Mechanisms in Strained Nanoislands

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The new mechanism for relaxation of misfit stresses in nanoislands (quantum dots) is suggested and theoretically examined which is the formation of partial misfit dislocations. The parameters of nanoislands are estimated at which the generation of partial misfit dislocations is energetically favorable, with emphasis on the case of Ge/Si nanoislands. Different dislocation structures are shown to be energetically preferred in different regions of the interface.

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The strain-driven formation of spatially ordered ensembles of nanoislands recently attracted tremendous attention motivated by their wide applications in nanotechnologies; see, e.g., [1–15]. Self-assembled semiconductor nanoislands (quantum dots) exhibit unique functional properties exploited in electronic and optoelectronic devices. From an applications viewpoint, desired functional characteristics of quantum dots crucially depend on their structure and geometry. In particular, the formation of misfit dislocations (MDs) in quantum dots leads to dramatic degradation of their functional properties. In this context, knowledge of critical geometric parameters of quantum dots, at which the formation of MDs is energetically favorable, is of utmost importance for applications of such dots. In addition to the technologically motivated attention to a theoretical description of defects in nanoislands (quantum dots), the behavioral features of nanoislands with defects are highly interesting for understanding the fundamentals of nanoscale effects in solids.

The geometry of a freestanding nanoisland opens up several modes of stress relaxation that are geometrically forbidden or energetically unfavorable in continuous thin films. In particular, lateral free surfaces of a freestanding nanoisland are capable of playing the crucial role in strain relaxation. Actually, in contrast to the situation with continuous thin films, MDs can be effectively generated at nodes of the lateral free surfaces of a nanoisland and the flat surface of either the substrate (Fig. 1) or the wetting layer, where crystallographic and energetic conditions of the dislocation formation are favorable. The main aim of this paper is to suggest and theoretically examine a new physical mechanism for strain relaxation in nanoislands, associated with their specific geometry, which is the generation of partial MDs at the lateral node points (Figs. 1c and 1d).

Let us consider a model composite solid consisting of a semi-infinite crystalline substrate and a pyramidlike crystalline nanoisland characterized by the base length L and the contact angle α of its free surface with the substrate (Fig. 1a). The nanoisland and substrate are assumed to be isotropic solids having the same values of the shear modulus G and the same values of Poisson ratio ν. For simplicity, hereafter we confine our consideration to the situation with the nanoisland/substrate boundary having a one-dimensional misfit characterized by the misfit parameter $f = 2(a - a_s)/(a + a_s)$, where a and a_s are the crystal lattice parameters of the nanoisland and the substrate, respectively.

Misfit stresses occur in the nanoisland due to the geometric mismatch characterized by f at the interphase boundary between the nanoisland and the substrate. The standard micromechanism for a partial relaxation of the misfit stresses in nanoislands and conventional films is treated to be the generation of perfect MDs (Fig. 1b) and their ensembles, respectively; see, e.g., [1,13–21]. In conventional films of nanoscale thickness, however, partial MDs are capable of being generated and causing relaxation of misfit stresses; see experimental data [22,23] and models [24]. With this taken into account, we address this paper on relaxation of misfit stresses via generation

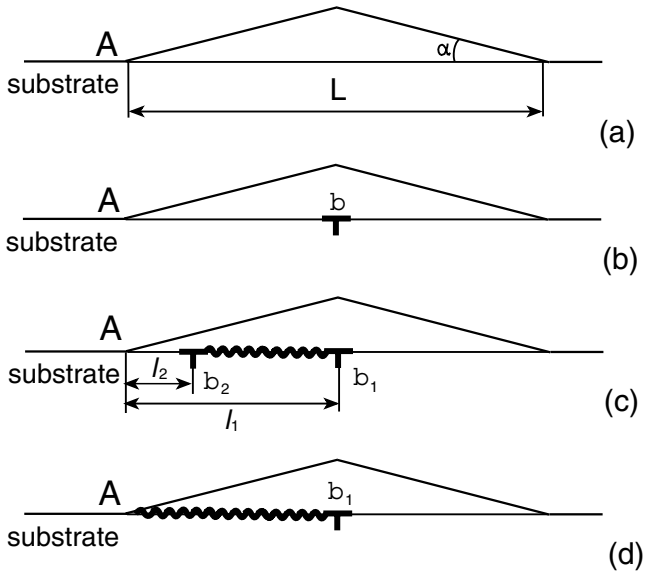

FIG. 1. Nanoisland/substrate boundary structures. (a) Coherent (dislocationfree) boundary. Semicoherent boundary with (b) one perfect misfit dislocation, (c) two partial misfit dislocations, and (d) one partial misfit dislocation.

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of partial MDs (associated with stacking faults) at the lateral node points of the nanoisland and their consequent motion along the island base [Figs. 1c and 1d].

Let us analyze the conditions at which the formation of partial MDs at the interphase boundary are energetically favorable in a nanoisland. To do so, we will compare energetic characteristics of the four following physical states realized in a composite solid: the coherent state with MD-free interphase boundary (Fig. 1a) and the three semicoherent states with the interphase boundary containing one perfect MD (Fig. 1b), two partial MDs (Fig. 1c), and one partial MD (Fig. 1d). The composite in the coherent, MD-free state (Fig. 1a) is characterized by the total elastic energy (per unit length) W_C being equal to the misfit strain energy W^f related to misfitting at the interphase boundary.

Let us consider the energies that characterize the semicoherent states (Figs. 1b–1d) of the interphase boundary. In doing so, we will start with estimation of the energy W_{2P} of the semicoherent state with two partial MDs (with a stacking fault between them; see Fig. 1c) at the nanoisland base. The energies W_L and W_{1P} which characterize the semicoherent states with one perfect, lattice MD (Fig. 1b) and one partial MD (Fig. 1d), respectively, can be found from the formula for the energy W_{2P} at some fixed values of parameters that specify the semicoherent state with two partial MDs.

The energy W_{2P} consists of the following six terms: $W = W^f + W^d + W^{\rm dc} + W^{f-d} + W^{d-d} + W^\gamma$. Here W^d denotes the proper elastic energy of the partial MDs, $W^{\rm dc}$ the energy of MD cores, W^{f-d} the elastic energy associated with the elastic interaction between the misfit stresses and the partial MDs, W^{d-d} the elastic energy that characterizes the elastic interaction between the MDs, and W^γ the energy of the stacking fault that joins the partial MDs (Fig. 1c). The state with the two partial MDs (Fig. 1c) is more energetically favorable than the coherent state (Fig. 1a), if

$$\Delta W_{2P-C} = W_{2P} - W_C = W^d + W^{\rm dc} + W^{f-d} + W^{d-d} + W^\gamma < 0. \quad (1)$$

In order to specify formulas for the energies figuring in formula (1), we should take into account the effects of nanoisland lateral free surfaces that provide the effective screening of MD stress fields due to the image forces. For definiteness and shortness, we will focus our consideration on the case of Ge/Si(100) nanoislands that have the great technological potential. Such nanoislands of the pyramid shape are bounded by {510} facets making a contact angle α of 11° with the [100] substrate [12]. With a low value of α taken into account, here we will characterize in the first approximation the screening effect caused by the nanoisland free surfaces, using formulas that describe the energetic characteristics of dislocations near flat free surfaces. In these formulas, the interspacing between a dislocation and the flat free surface will be replaced by that between a dislocation and the nearest lateral free surface of the dislocated nanoisland. That is, a MD distant by d from the nearest lateral free surface of the nanoisland is considered in our approximate calculations as a dislocation distant by d from the flat free surface of a semi-infinite solid (Fig. 2a). Since the contact angle α is small, the nanoisland free surface curvature causes a detectable influence on the MD stress fields in only the situation where the MD is located in the vicinity of the center point B of the nanoisland base. This influence will be estimated below as that of a cylinder free surface (Fig. 2b).

With the approximation discussed (Fig. 2a), the proper energy of the two MDs can be written as follows:

$$W^d \approx \frac{Gb_1^2}{4\pi(1-\nu)} \ln\left(\frac{R_1}{r_1}\right) + \frac{Gb_2^2}{4\pi(1-\nu)} \ln\left(\frac{R_2}{r_2}\right), \quad (2)$$

where b_i, R_i, and $r_i (r_i \approx b_i)$ are, respectively, the magnitude of the Burgers vector, the screening length of stress fields, and the core cutoff radius of the ith partial MD ($i = 1, 2$). Following the analysis of dislocation stress fields near flat free surfaces [25], the screening length R_i of the stress fields induced by the ith partial MD is taken as the double distance d_i between the ith MD and the nearest free surface of the pyramidlike nanoisland. That is, $R_i = 2d_i$, where

$$d_i = \begin{cases} l_i \sin\alpha, & \text{if } l_i \le L/2 \\ (L - l_i)\sin\alpha, & \text{if } l_i > L/2, \end{cases} \quad (3)$$

with l_i being the interspacing between the ith partial MD and the lateral node point A (Fig. 1c).

With the approximation discussed above, the energy that characterizes the elastic interaction between the misfit stresses and the MDs is given as

$$W^{f-d} \approx -2Gf(b_1 d_1 + b_2 d_2)(1+\nu)/(1-\nu). \quad (4)$$

The energy associated with the elastic interaction between the partial MDs (calculated as that between dislocations located near the flat free surface) is given as [26]

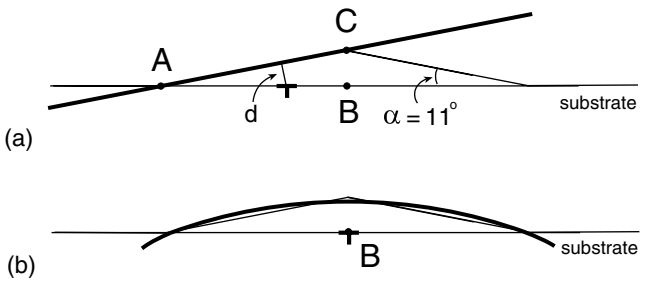

FIG. 2. The screening effect of the nanoisland free surface on dislocation stress fields is modeled as that of (a) straight free surface (solid line AC); or (b) cylinder free surface (solid curve).

$$W^{d-d} = \frac{Gb_1b_2}{4\pi(1-\nu)}\left\{1 + \frac{2(l_1-l_2)^2}{(l_1-l_2)^2+(d_1-d_2)^2} + \frac{8d_1d_2(l_1-l_2)^2}{[(l_1-l_2)^2+(d_1+d_2)^2]^2} - \frac{2(l_1-l_2)^2+4d_1d_2}{(l_1-l_2)^2+(d_1+d_2)^2} + \ln\left[\frac{(l_1-l_2)^2+(d_1+d_2)^2}{(l_1-l_2)^2+(d_1-d_2)^2}\right]\right\}. \quad (5)$$

For $(\sin\alpha)^2 \ll 1$ [it is the case of Ge/Si(100) nanoislands], from Eqs. (3) and (5) we find the following approximate formula for W^{d-d}:

$$W^{d-d} \approx \frac{Gb_1b_2}{4\pi(1-\nu)}\left\{3 + \frac{8d_1d_2(l_1-l_2)^2}{[(l_1-l_2)^2+(d_1+d_2)^2]^2} - \frac{2(l_1-l_2)^2+4d_1d_2}{(l_1-l_2)^2+(d_1+d_2)^2} + \ln\left[1+\frac{4d_1d_2}{(l_1-l_2)^2}\right]\right\}. \quad (6)$$

The energy W^{dc} of MD cores in the standard approximation [27] is given as

$$W^{dc} \approx \frac{G}{4\pi(1-\nu)}(b_1^2+b_2^2). \quad (7)$$

Finally, the energy of the stacking fault formed between the two partial MDs (Fig. 1c) is $W^{\gamma} \approx \gamma(l_1-l_2)$, where γ denotes the energy density of the stacking fault (per its unit area).

With this relationship and formulas (1)–(4), (6), and (7), we find the following formula for ΔW_{2P-C}:

$$\Delta W_{2P-C}(l_1,l_2) \approx \frac{G}{4\pi(1-\nu)}\left\{b_1^2\left[\ln\left(\frac{2d_1}{r_1}\right)+1\right] + b_2^2\left[\ln\left(\frac{2d_2}{r_2}\right)+1\right] - 8\pi f(1+\nu)(b_1d_1+b_2d_2) + \frac{4\pi\gamma(1-\nu)}{G}(l_1-l_2)\right\} + W^{d-d}(l_1,l_2). \quad (8)$$

For $\Delta W_{2P-C} < 0$, the state with the two partial MDs (Fig. 1c) in nanoislands is more energetically favorable than the coherent state (Fig. 1a). In this situation, the equilibrium interspacing λ_0 between the two partial MDs [characterized by the coordinate $(l_1+l_2)/2$ of the stacking fault center located between them] corresponds to a minimum value of ΔW_{2P-C} as a function of $\lambda = l_1 - l_2$ at a given value of $(l_1+l_2)/2$.

Now let us consider the state of a nanoisland with one partial MD (Fig. 1d). The difference ΔW_{1P-C} between the energies of the nanoisland with one partial MD (Fig. 1d) and the coherent state of the nanoisland (Fig. 1a) is given as

$$\Delta W_{1P-C} = \Delta W_{2P-C}(b_1 < a, b_2 = 0, l_2 = 0). \quad (9)$$

In general, as with partial MDs, perfect MDs (Fig. 1b) can be generated in nanoislands. The difference ΔW_{L-C} between the energies of the nanoisland with one perfect lattice MD (Fig. 1b) and a MD-free nanoisland (Fig. 1a), in our approximation, is given as

$$\Delta W_{L-C} = \Delta W_{2P-C}(b_1 = a, b_2 = 0, l_1 = l_2). \quad (10)$$

Comparison of the characteristic energies ΔW_{2P-C}, ΔW_{1P-C}, and ΔW_{L-C} 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 $\Delta W_{2P-C}|_{\lambda=\lambda_0}$, ΔW_{1P-C}, and ΔW_{L-C} on z. Here, z is the coordinate of, respectively, the perfect MD ($z = l_1$) and the partial MD ($z = l_1$) in the cases shown in Figs. 1b and 1d, respectively; and z is the coordinate of the stacking fault center [$z = (l_1+l_2)/2$] in the case of two partial MDs (Fig. 1c). The calculated dependences are presented in Fig. 3, for Ge/Si(100) nanoislands characterized by the following values of parameters: $f = 0.042$, $a = 0.566$ nm, $L = 100a$, $\gamma = 6.9 \times 10^{-2}$ J m^{-2}, $G = 40$ GPa, $\nu = 0.26$. In doing so, curves 1, 2, and 3 in Fig. 3 correspond to dependences of, respectively, $\Delta W_{2P-C}(\lambda = \lambda_0, b_1 = b_2 = a/2)$, $\Delta W_{1P-C}(b_1 = a/2)$, and ΔW_{L-C} on z. The dependence $\lambda_0(z)$ is shown in Fig. 3 as a solid curve.

For a given value of z, the lowest dependence from the set $(\Delta W_{2P-C}|_{\lambda=\lambda_0}, \Delta W_{1P-C}, \Delta W_{L-C})$ of dependences shown in Fig. 3 specifies the most energetically favorable MD configuration at this value of z. As it follows from Fig. 3, a single partial MD (Fig. 1d) is not favorable at any z. In the range of z/L from 0.03 to 0.36 and from 0.64 to 0.97, the two partial MDs (Fig. 1c) are characterized by the minimum energy. In most of this range, the suggested model approximation (Fig. 2a) is effective, because MDs are located in the vicinity of the nearest straight lateral free surface and are far enough from other segments of the nanoisland free surface. In the range of z/L from 0.36 to 0.64, the perfect MD (Fig. 1b) is energetically favorable.

Notice that the model used in this paper is too approximate to make strict conclusions on the MD type in the range of z/L from 0.01 to 0.03 and from 0.97 to 0.99. Also, the nanoisland free surface curvature causes a detectable effect on stress fields of MDs located in vicinity of the nanoisland base center B. In the first approximation, the curvature effect can be estimated using the results of paper [21] describing the generation of MDs in cylindrical composites. In doing so, with the effect of a pyramid top free surface curvature modeled as that of a cylinder free surface characterized by cylinder radius $0.5L\cot 11°$ (see Fig. 2b) and with Eqs. (26) and (28) of paper [21],

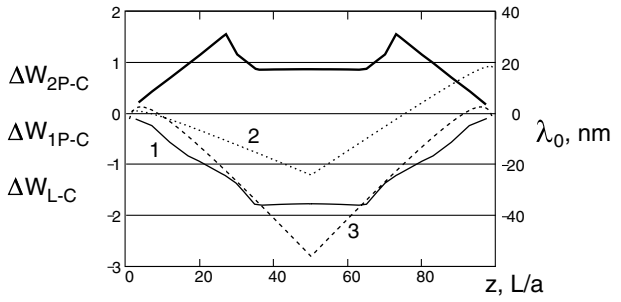

FIG. 3. Dependences of the energetic characteristics (in units of $\frac{G}{4\pi(1-\nu)}$), ΔW_{2P-L} (curve 1), ΔW_{1P-L} (dotted curve 2), and ΔW_{L-C} (dashed curve 3), of a Ge/Si(100) nanoisland on dislocation configuration coordinate z (see text). Dependence $\lambda_0(z)$ is shown as a solid curve.

we find that the perfect MD is energetically unfavorable compared to even the coherent state. A detailed analysis of the free surface curvature effect on MDs located in the vicinity of the base center B is beyond the scope of this Letter. In any event, however, results of this analysis will not change dramatically our conclusion that formation of the partial MDs (Fig. 1c) is 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 commonly are 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 MDs 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 MDs is more spatially homogeneous, compared to that created by a perfect MD. 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 MDs and the conventionally modeled case with a perfect MD.

Thus, in this paper the new relaxation mechanism in strained nanoislands—the generation of partial MDs at the lateral node points (Figs. 1c and 1d)—has been suggested. According to our theoretical analysis, the generation of partial MDs effectively competes with that of conventional perfect MDs, depending on structural and geometric characteristics of nanoislands. 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 [28,29], bulk semiconductors [30], and superconductors [31,32].

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[1] V. A. Shchukin and D. Bimberg, Rev. Mod. Phys. **71**, 1125 (1999).
[2] N. N. Ledentsov *et al.,* Semiconductors **32**, 343 (1998).
[3] J. A. Floro *et al.,* Phys. Rev. Lett. **84**, 701 (2000).
[4] P. Sutter and M. G. Lagally, Phys. Rev. Lett. **84**, 4637 (2000).
[5] A. Bourett, Surf. Sci. **432**, 32 (1999).
[6] N. Liu *et al.,* Phys. Rev. Lett. **84**, 334 (2000).
[7] C.-P. Liu *et al.,* Phys. Rev. Lett. **84**, 1958 (2000).
[8] D. E. Jesson, M. Kästner, and B. Voigtländer, Phys. Rev. Lett. **84**, 330 (2000).
[9] T. I. Kamins *et al.,* J. Appl. Phys. **81**, 211 (1997).
[10] S. A. Chaparro *et al.,* Phys. Rev. Lett. **83**, 1199 (1999).
[11] S. A. Chaparro, Y. Zhang, J. Drucker, and D. J. Smith, Appl. Phys. **87**, 2245 (2000).
[12] J. Tersoff, C. Teichert, and M. G. Lagally, Phys. Rev. Lett. **76**, 1675 (1996).
[13] E. Pehlke, N. Moll, A. Kley, and M. Scheffler, Appl. Phys. A **65**, 525 (1997).
[14] H. T. Johnson and L. B. Freund, J. Appl. Phys. **81**, 6081 (1997).
[15] R. V. Kukta and L. B. Freund, J. Mech. Phys. Solids **45**, 1835 (1997).
[16] J. H. van der Merve, Crit. Rev. Solid State Mater. Sci. **17**, 187 (1991).
[17] S. C. Jain, J. R. Willis, and R. Bullough, Adv. Phys. **39**, 127 (1990).
[18] E. A. Fitzgerald, Mater. Sci. Rep. **7**, 87 (1991).
[19] S. C. Jain, A. H. Harker, and R. A. Cowley, Philos. Mag. A **75**, 1461 (1997).
[20] I. A. Ovid'ko, J. Phys. Condens. Matter **11**, 6521 (1999); **13**, L97 (2001).
[21] M. Yu. Gutkin, I. A. Ovid'ko, and A. G. Sheinerman, J. Phys. Condens. Matter **12**, 5391 (2000).
[22] M. Loubradou, R. Bonnet, A. Vila, and P. Ruterana, Mater. Sci. Forum. **207–209**, 285 (1996).
[23] M. Tamura, Appl. Phys. A **63**, 359 (1996).
[24] M. Yu. Gutkin, K. N. Mikaelyan, and I. A. Ovid'ko, Phys. Solid State **40**, 1864 (1998); **43**, 42 (2001).
[25] V. I. Vladimirov, M. Yu. Gutkin, and A. E. Romanov, Poverkhnost **6**, 46 (1988).
[26] I. A. Ovid'ko and A. G. Sheinerman (to be published).
[27] J. P. Hirth and J. Lothe, *Theory of Dislocations* (Wiley, New York, 1982).
[28] I. A. Ovid'ko, Mater. Sci. Eng. A **154**, 29 (1992).
[29] D Gaillard *et al.,* Phil. Mag. A **80**, 237 (2000).
[30] J. R. K. Bigger *et al.,* Phys. Rev. Lett. **69**, 2224 (1994).
[31] I.-Fei Tsu, S. E. Babcock, and D. L. Kaiser, J. Mater. Res. **11**, 1383 (1996).
[32] M. Yu. Gutkin and I. A. Ovid'ko, Phys. Rev. B **63**, 064515 (2001).