

# NANO-ISLANDS ON PLASTICALLY DEFORMED SUBSTRATES WITH DISCLINATIONS

I.A. Ovid'ko and A.G. Sheinerman

Institute for Problems of Mechanical Engineering, Russian Academy of Sciences, Bolshoj 61, Vas. Ostrov, St.Petersburg, 199178, Russia

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**Abstract.** Spatial arrangements of nano-islands deposited on plastically deformed substrates containing wedge disclinations (defects of rotational type) are theoretically examined. It is shown that the elastic interaction between the nano-islands and the disclinations is capable of causing preferable spatial positions of nano-islands. The parameters of the substrate/nano-island systems are theoretically revealed that control spatial positions of nano-islands on disclinated substrates.

## 1. INTRODUCTION

The strain-driven formation of spatially ordered ensembles of nano-islands recently attracted tremendous attention motivated by the interest to their wide applications in nanotechnologies; see, e.g. [1-14]. Of special importance are applications of self-assembled semiconductor nano-islands (quantum dots) exhibiting unique functional properties exploited in electronic and optoelectronic applications. In doing so, desired, from an applications viewpoint, spatial order of nano-island ensembles comes into play owing to the elastic interaction between nano-islands (see reviews [1-3]). Recently, a promising technological method for fabrication of spatially ordered ensembles of quantum dots has been suggested and theoretically examined in papers [15,16], which is the formation of nano-islands (quantum dots) on free surfaces of substrates with internal interphase or low-angle grain boundaries. This method exploits the idea to control spatial organization of arrays of nano-islands by means of the elastic interaction between nano-islands and ordered networks of dislocations at the internal boundaries.

We think that the method under consideration can be treated as a partial case of the general technological approach which deals with a human-controlled modification of substrates in order to fabricate films and nano-island ensembles (on sub-

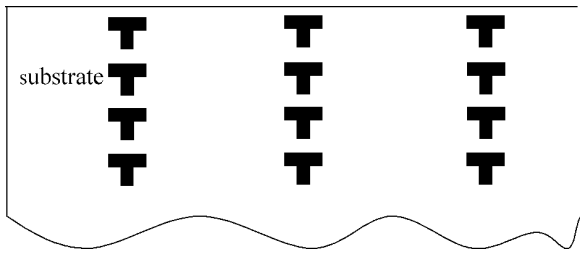
strates) with desired functional properties. In this context, a promising method to modify substrates, which is another partial case of the general approach discussed, is plastic deformation of substrates. Actually, plastic deformation processes are capable of creating internal sources of stresses in a substrate that influence spatial positions of nano-islands on the substrate free surface due to elastic interaction between the nano-islands and the stress sources. In doing so, the stress sources – defect configurations – in plastically deformed solids often form spatially ordered structures which, therefore, can give rise to the formation of spatially ordered ensembles of nano-islands on the free surfaces of pre-deformed substrates. The main aim of this paper is to theoretically examine the behavior of nano-islands on plastically deformed substrates that contain disclinations (defect of rotational type) generated under mechanical load.

## 2. FORMATION OF DISCLINATIONS IN PLASTICALLY DEFORMED SUBSTRATES

Dislocation walls (low-angle grain boundaries), which have a rather regular spatial arrangement, are often formed in crystalline solids under plastic deformation [17, 18]. If such deformation-induced dislocation walls are generated in a deformed substrate, they can cause spatial ordering of nano-islands

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Corresponding author: I.A. Ovid'ko, e-mail: ovidko@def.ipme.ru

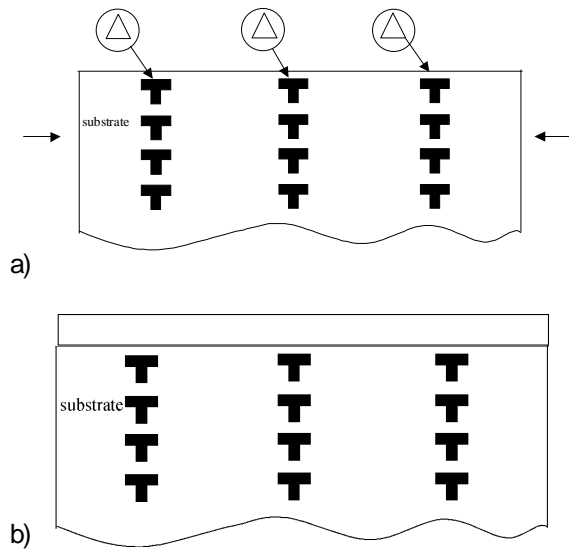


**Fig. 1.** Dislocation walls in plastically deformed substrate are terminated by stress sources of disclination type.

deposited on the substrate. In order to quantitatively examine this phenomenon, we should specify stress fields created by dislocation walls on the substrate free surface. The deformation-induced dislocation walls are, in general, ragged (Fig. 1). That is, the “end” dislocation belonging to a dislocation wall and being closest to the substrate free surface is distant by  $H (>0)$  from the free surface (Fig. 1). The “end” dislocation of a ragged dislocation wall serves as a stress source of disclination type, or, in short, as a disclination [18]. The stress field created by the disclination on the substrate free surface dominates over any other contributions to the stress field created by a dislocation wall on the free surface. In these circumstances, the effects of deformation-induced dislocation walls on spatial arrangement of nano-islands on the substrate free surface, in the first approximation, can be described as those associated with stress fields of the disclinations.

In the following sections of this paper we will theoretically examine the influence of the disclinations on the characteristics of nano-island ensembles on the substrate free surface with some assumptions (that simplify the theoretical analysis) taken into consideration. In particular, the disclinations are assumed to be identical and form regular orthogonal rows equally distant from the free surface. The consideration under simplifying assumptions will allow us to reveal the key specific features of nano-island ensembles on disclinated substrates and will serve as a basis for further, more detailed examinations of nano-islands deposited on plastically deformed substrates.

Finally, it should be noted that the distance between disclination rows and the substrate free surface can be regulated in the following two-step manner. At the first step, the substrate is plastically deformed, in which case low-angle grain boundaries are formed (Fig. 2a). At the second step, a new layer of a technologically controlled thickness



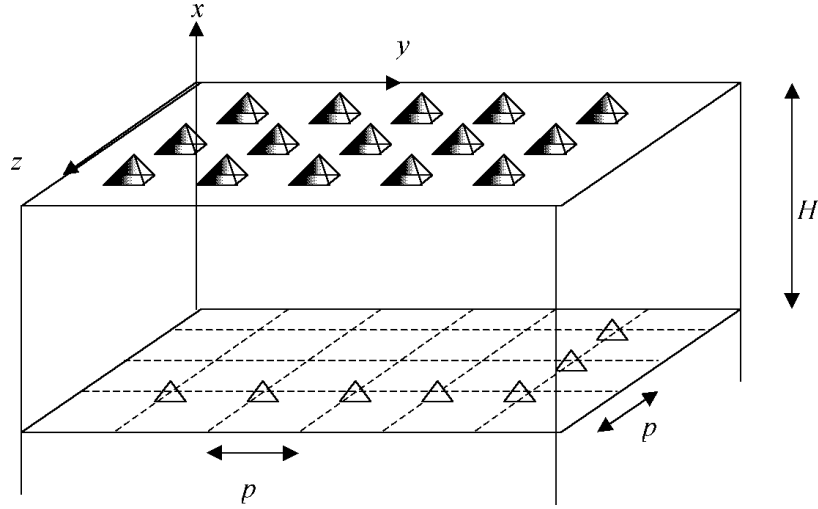
**Fig. 2.** Formation of disclinations in substrate – (a) Plastic deformation of substrate, (b) Deposition of layer on plastically deformed substrate.

is deposited on the deformed substrate (Fig. 2b). The aforesaid method allows one to synthesize a composite substrate with the controlled minimum thickness between disclinations and the substrate free surface.

### 3. NANO-ISLANDS ON DISCLINATED SUBSTRATES. MODEL

Let us consider a model composite system consisting of an elastically isotropic semi-infinite substrate 1 and elastically isotropic pyramid-like nano-islands 2 (Fig. 3). The shear modulus  $G$  and the Poisson ratio  $\nu$  are assumed to be identical for the substrate and the nano-islands. For definiteness, hereafter we confine our examination to the situation with cubic crystal lattices of the substrate and the nano-islands. In these circumstances, the interphase boundaries between the substrate and the nano-islands are characterized by the two-dimensional dilatation misfit  $f=2(a_1-a_2)/(a_1+a_2)$ , where  $a_1$  and  $a_2$  are the crystal lattice parameters of the substrate and the nano-islands, respectively. The disclination ensemble in the substrate is modeled by the two infinite orthogonal rows of periodically arranged disclinations (Fig. 3) characterized by a strength  $\omega$  and distant by  $H$  from the substrate free surface. The spacing between neighboring parallel disclinations (period) is designated by  $p$ .

Let us calculate equilibrium positions of nano-islands on a disclinated substrate. In general, equi-



**Fig. 3.** Nano-islands on substrate with disclination network consisting of two infinite orthogonal rows of wedge disclinations.

librium positions of nano-islands on a substrate are defined as those corresponding to the minimum elastic energy density of a system. The energy density includes both the terms depending on the spatial positions of nano-islands and the terms independent on such positions. The former terms are related to both interaction of nano-islands with stress fields induced by stress sources in the substrate and island/island interaction. In this paper we focus our consideration on disclinations as stress sources in the substrate, that influence spatial positions of nano-islands. In doing so, in the first approximation, we consider the situation where the spacing between neighboring nano-islands is close to that between neighboring disclinations. This situation occurs when adatoms (composing the nano-island phase) have high mobility at the substrate free surface; they easily move to those sites at the disclination-stressed surface that are favorable for nucleation of nano-islands. In the situation discussed, the island/island interaction is negligible because nano-islands create short-range stress fields. Also, in our first approximation analysis we will neglect the interaction of disclinations with nano-island-induced stress fields.

With the aforesaid assumptions, equilibrium positions of nano-islands are those corresponding to a minimum of the elastic energy  $W$  of each nano-island. The energy  $W$  can be written as follows [16]:

$$W = w_0 R\left(\frac{c}{l}\right) V, \quad (1)$$

where  $w_0$  denotes the elastic energy density (per unit volume) of a nano-island, which does not take into account its relaxation\*;  $V$  is the nano-island volume; and  $R(c/l)$  is the shape factor depending on the ratio  $c/l$  of the nano-island height to its base length.

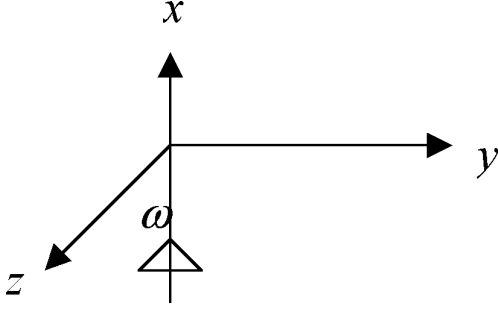
To calculate  $w_0$ , we need formulae for strain fields created by two rows of disclinations (Fig. 3) on the substrate free surface. These formulae will be derived in the next section.

#### 4. DISLOCATION-INDUCED STRAINS ON SUBSTRATE FREE SURFACE

Let us calculate strains induced by disclination rows (Fig. 3) at the substrate free surface. To do so, we will use the following known [18] formula for the stress created by a wedge disclination with strength  $\omega$  and the disclination line core distant by  $H$  from the free surface (Fig. 4):

$$\sigma_{yy}(x, y) = \frac{G\omega}{2\pi(1-\nu)} \left\{ \frac{1}{2} \frac{(x+H)^2 + y^2}{(x-H)^2 + y^2} + \frac{(x+H)^2}{(x+H)^2 + y^2} - \frac{(x-H)^2}{(x-H)^2 + y^2} + \frac{2H[(x-H)^2(2H-x) + y^2(2H-3x)]}{[(x-H)^2 + y^2]^2} \right\}. \quad (2)$$

\* In other words,  $w_0$  is the energy density of a nano-island treated as a fragment of a thin film.



**Fig. 4.** Wedge disclination in semi-infinite elastic medium.

There is one non-zero component,  $\varepsilon_{yy}(y)$ , of the tensor of strain created by such a disclination at the free surface, which entails from formula (2) and Hooke's law as follows:

$$\varepsilon_{yy}(y) = \frac{\sigma_{yy}(0, y)}{2(1+\nu)G} = \frac{\omega}{\pi(1-\nu^2)} \frac{H^2}{y^2 + H^2}. \quad (3)$$

Now let us consider strains,  $\varepsilon_{yy}^{(1)}(y)$  and  $\varepsilon_{zz}^{(2)}(z)$ , created by rows of disclinations with strength  $\omega$  and line cores ( $x=0, y=np$ ) and ( $x=0, z=np$ ), where  $n$  is integer (Fig. 3). The strains in question can be calculated as the sums of the strains (given by formula (3)) created by isolated disclinations belonging to the orthogonal rows. In doing so, we get:

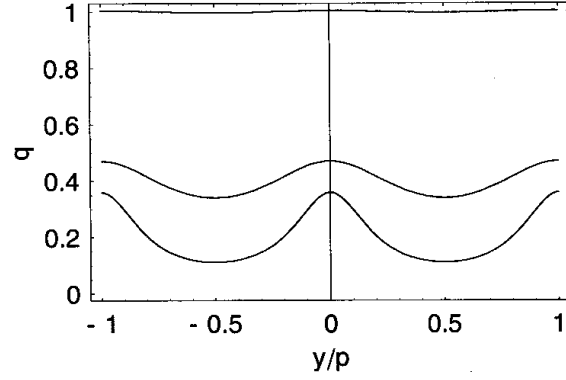
$$\varepsilon_{yy}^{(1)}(y) = \frac{\omega H^2}{\pi(1-\nu^2)} \sum_{n=-\infty}^{\infty} \frac{1}{(y-np)^2 + H^2} = \frac{\omega}{1-\nu^2} q\left(\frac{y}{p}\right), \quad (4)$$

$$\varepsilon_{zz}^{(2)}(z) = \varepsilon_{yy}^{(1)}(z) = \varepsilon^{ar}(z), \quad (5)$$

where

$$q(t) = \frac{H}{p} \frac{\sinh\left(\frac{2\pi H}{p}\right)}{\cosh\left(\frac{2\pi H}{p}\right) - \cos(2\pi t)}. \quad (6)$$

For illustration, the dependences  $q(y/p)$  are presented in Fig. 5, for various values of the parameter  $H/p$ . The minimums and the maximums of the function  $q(y/p)$  are located at the points  $y = p(n+1/2)$  and  $y = np$ , respectively. The maximum and the minimum values,  $q_{max}$  and  $q_{min}$ , of the function  $q(t)$  are respectively as follows:



**Fig. 5.** Dependences of parameter  $q$  on non-dimensional coordinate  $y/p$ , for  $H/p=1$ ,  $H/p=0.4$ , and  $H/p=0.2$  (from top to bottom).

$$q_{min} = \frac{H}{p} \tanh \frac{\pi H}{p}, \quad (7)$$

$$q_{max} = \frac{H}{p} \coth \frac{\pi H}{p}. \quad (8)$$

In the limiting case with  $H/p \ll 1$ , we have  $q_{min} \approx 0$  and  $q_{max} \approx 1/\pi$ .

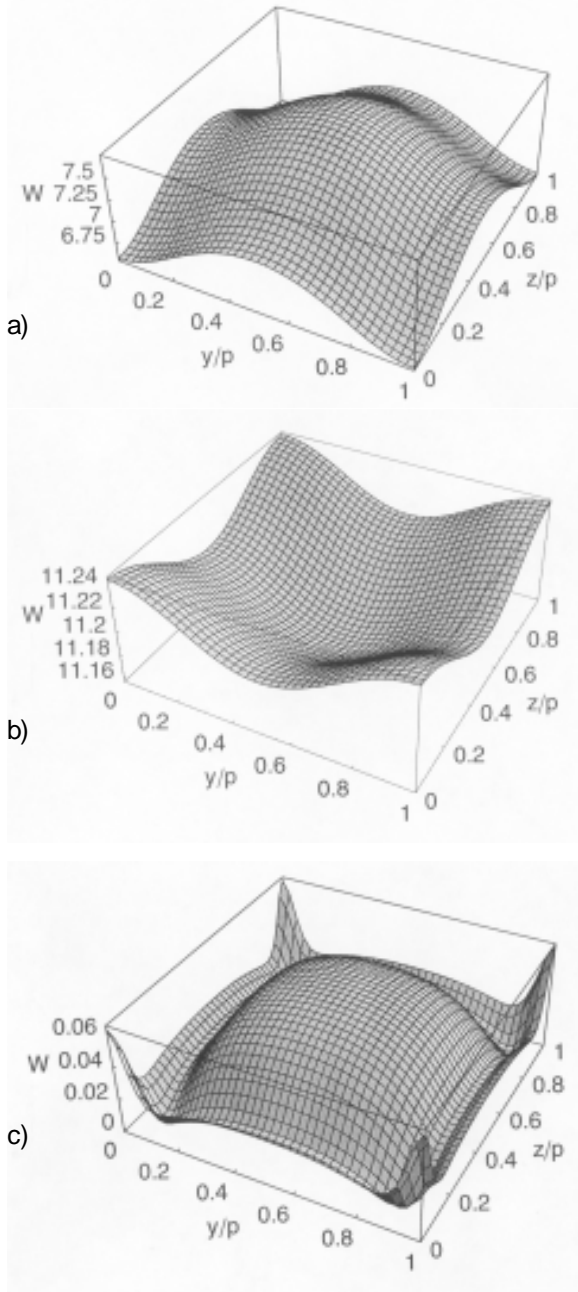
## 5. ELASTIC ENERGY AND EQUILIBRIUM POSITIONS OF NANO-ISLANDS

In order to calculate  $W$  and analyze its minimums (corresponding to equilibrium positions of nano-islands), first, let us calculate the elastic energy density  $w_0$  of nano-islands, that does not take into account their relaxation. In the discussed situation with an in-plane stressed solid (nano-islands are treated as fragments of a thin film), we have:

$$w_0 = \frac{G}{1-\nu} \left[ (\varepsilon_{yy}^f(y))^2 + 2\nu \varepsilon_{yy}^f(y) \varepsilon_{zz}^f(z) + (\varepsilon_{zz}^f(z))^2 \right], \quad (9)$$

where  $\varepsilon_{yy}^f(y) = \varepsilon^{ar}(y) + f$  and  $\varepsilon_{zz}^f(z) = \varepsilon^{ar}(z) + f$ .

The surfaces  $W(y, z) = w_0 R(d/l) V$  (in units of  $G\omega^2 R(d/l) V / [(1-\nu^2)^2(1-\nu)]$ ) are shown in Fig. 6, for various values of the parameters  $p/H$  and  $(1-\nu^2)f/\omega$ . From Fig. 6 it follows that the points of minimums of  $w_0(y, z)$  (and, therefore,  $W(y, z)$ ) are located under diagonal lines of the disclination network at the lines  $y = z \pm np$ . These points are located either under the nodes of the disclination network (Fig. 6a) or under the centers of the disclination network squares (Fig. 6b) or under other points of diagonal lines (Fig. 6b,c) depending on values of parameters  $p/H$  and  $(1-\nu^2)f/\omega$ . From Fig. 6 it follows that the rate of change of



**Fig. 6.** Energy  $W$  (in units of  $G\omega^2 R(c/l) V / [(1-\nu^2)^2(1-\nu)]$ ) accumulated in nano-islands as a function of nano-island coordinates  $x$  and  $y$ , for  $\nu = 0.4$ , (a)  $(1-\nu^2)f/\omega = -2$ ,  $H/p = 0.4$ ; (b)  $(1-\nu^2)f/\omega = 1$ ,  $H/p = 1$ ; and (c)  $(1-\nu^2)f/\omega = -0.18$ ,  $H/p = 0.1$ .

the nano-island energy  $W(x, y)$  at large values of  $H/p$  is low, which results in a low value of the force that acts on the nano-island. This increases the probability of the nano-islands to be shifted from their equilibrium positions.

From the condition  $y_{eq} = \pm z_{eq} - np$  and formulae (4)-(6), we find that  $\varepsilon^{ar}(y_{eq}) = \varepsilon^{ar}(z_{eq})$  and, as a

corollary, the function  $w_0$  at the points  $(y_{eq}, z_{eq})$  of its minimums can be written as follows:

$$w_0(y_{eq}, z_{eq}) = 2G \frac{1+\nu}{1-\nu} (\varepsilon^{ar}(y_{eq}) + f)^2 = 2G \frac{1+\nu}{1-\nu} \frac{\omega^2}{(1-\nu^2)^2} \left( q\left(\frac{y_{eq}}{p}\right) + \frac{(1-\nu^2)f}{\omega} \right)^2. \quad (10)$$

Formula (10) gives the conditions at which nano-islands are located at points under the centers or nodes of the disclination network cells (squares) or at some intermediate points under diagonal lines of the disclination network. So, there are the following situations depending on the parameters  $H/p$  and  $(1-\nu^2)f/\omega$ :

- (i)  $q_{min} + f(1-\nu^2)/\omega > 0$ , that is,  $f/\omega > 0$  or  $(f/\omega < 0$  and  $\gamma > 1/q_{min})$ , where  $\gamma = \omega/[f(1-\nu^2)]$ . In this situation, the points of minimum of  $w_0$  coincide with the points  $y = p(n+1/2)$  of minimum of  $q(y/p)$ ; the equilibrium positions of the nano-islands are located under the centers of the disclination network cells.
- (ii)  $q_{max} + f(1-\nu^2)/\omega < 0$ , that is,  $f/\omega < 0$  and  $\gamma < 1/q_{max}$ . In this situation, the points of minimum of  $w_0$  coincide with the points  $y = np$  of maximum of the function  $g(y/p)$ ; the equilibrium positions of the nano-islands are located under the nodes of the disclination network cells.
- (iii)  $f/\omega < 0$  and  $1/q_{max} < \gamma < 1/q_{min}$ . In this situation, the equilibrium positions  $y=z=y_0$  of nano-islands are located under the points of the diagonal lines of the disclination network, which satisfy the condition  $g(y_0/p) = -f(1-\nu^2)/\omega$ .

In Fig. 7 the state diagram of the system under consideration is shown in the coordinates  $(H/p, \gamma)$ . The regions I (with  $\gamma > 1/q_{min}(H/p)$ ), II (with  $1/q_{max}(H/p) < \gamma < 1/q_{min}(H/p)$ ) and III (with  $\gamma < 1/q_{max}(H/p)$ ) on the diagram correspond to the situations (i), (ii) and (iii), respectively.

The situations (i) and (ii), with nano-islands homogeneously distributed over the substrate free surface occur either at low values,  $|\omega| < \omega_{c1} = (1-\nu^2)f/q_{max}$ , of the disclination strength modulus  $|\omega|$  or at high values,  $|\omega| > \omega_{c2} = (1-\nu^2)f/q_{min}$ , of  $|\omega|$ ; see regions I and III in Fig. 7. The critical values of  $\omega_{c1}$  and  $\omega_{c2}$  decrease with increase of  $H/p$ . In doing so, regions I and III, which are characterized by a homogeneous distribution of nano-islands, expand. In the limiting case with  $H/p \rightarrow 0$ , we have:  $\omega_{c1} \rightarrow \pi(1-\nu^2)|f|$  and  $\omega_{c2} \rightarrow \infty$ . That is, the distribution of nano-islands is homogeneous only at low values of  $|\omega|$  ( $< \omega_{c1}$ ). For  $H/p \gg 1$ , we have:  $\omega_{c1} \rightarrow 0$  and  $\omega_{c2} \rightarrow 0$ , in which case

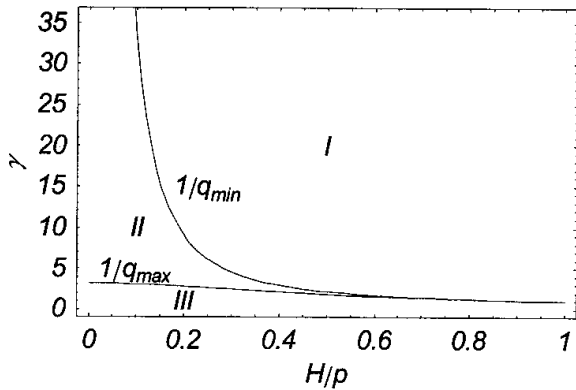


Fig. 7. Dependences of parameters  $q_{max}$  and  $q_{min}$  on  $H/p$ .

the distribution of nano-islands is homogeneous at any values of disclination strength  $\omega$ .

## 6. CONCLUDING REMARKS

In this paper we have theoretically described the influence of disclinations (that terminate dislocation walls) in plastically deformed substrates on the spatial arrangement of nano-islands deposited on the substrate. The influence in question results from the elastic interaction between the disclinations and the nano-islands. In the first approximation, deformation-induced disclination ensembles in substrates have been modeled as regular orthogonal rows of identical wedge disclinations equally distant from the substrate free surface (Fig. 3). In the framework of the model, it has been shown that nano-islands deposited on a disclinated substrate have preferable equilibrium spatial positions caused by interaction of the nano-islands with the stress fields of the disclinations. So, there are the following preferable positions of nano-islands depending on the parameters of the substrate/nano-island system: equilibrium positions of nano-islands are located under the (i) centers, (ii) nodes, (iii) diagonal lines of the disclination network cells (see Fig. 6). The aforesaid potentially allows one to design and fabricate nano-island ensembles with desired spatial arrangements (and, therefore, functional characteristics) using technologically controlled and/or influenced parameters (misfit parameter, distance between disclinations, etc.) of substrate/nano-island systems as an input.

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