Rev. Adv. Mater. Sci. (2003) 163-169

DEFECTS IN SQUARE 2D ARRAYS OF STRAINED QUANTUM DOTS

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

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

Received: May 22, 2003

Abstract. A theoretical model is suggested which describes quantum dot ensembles of the new type, namely the quantum dot arrays with defects. These defects represent local violations of the geometry of 2D arrays formed by quantum dots on crystalline substrates. The elastic moduli of strained arrays of quantum dots are estimated, in which case strains describe deviations of spatial positions of quantum dots from nodes of ideal square arrays. The formulas for characteristic energies of dislocations, disclinations and point defects in 2D arrays of quantum dots are derived. It is shown that point defects are characterized by comparatively low values of the formation energy and, therefore, are capable of being intensively formed in quantum dot arrays fabricated at highly non-equilibrium conditions.

1. INTRODUCTION

The rapidly growing scientific and technological interest in semiconductor nanoislands — quantum dots (QDs) — has arisen from the unique properties associated with their nanoscale structure and self-assembly; see, e.g., [1-16]. The outstanding optoelectronic properties of spatially ordered ensembles of QDs on crystalline substrates are the subject of intensive theoretical and experimental study due to both their use in device applications and significance for understanding the fundamentals of nanoscale effects in solids. Highly desired, from an applications viewpoint, functional characteristics of self-assembled QDs crucially depend on their spatial arrangement and distributions in size and form. In particular, free standing QDs commonly form a regular 2D array on the substrate free surface (due to elastic interactions between the dots [1,15] and/or between the dots and regularly arranged stress sources in the substrate [17-19]), in which case the geometry of the array of QDs strongly influences their properties. In this context, knowledge and control of geometric parameters of QD arrays are very important for fabrication and design of self-assembled QDs with desired functional characteristics.

QD arrays are conventionally described as ideal (defect-free) lattices with nodes occupied by QDs (Fig. 1 a); see, e.g., review article [1]. We think that, as with conventional crystalline lattices of solids, QD arrays may contain topological defects, such as dislocations (Fig. 1 b), disclinations (Fig. 1 c), vacancies and interstitial QDs (Fig. 1 d). In this event, the new geometry of defected arrays of QDs strongly affects the structure and properties of QDs. Actually, QD arrays with defects (Fig. 1 b,c and d) are characterized by irregularities in spatial arrangement of QDs at the defect cores and deviations of interspacing between QDs from that inherent to the ideal array shown in Fig. 1 a. Such irregularities and deviations cause the differences in the stress fields (sensitive to interspacing between QDs) in QDs and their vicinities in the situations with ideal (Fig. 1 a) and defected (Fig. 1 b,c and d) arrays. At the same time, the stress fields crucially influence the structure (in particular, formation of conventional misfit dislocations at interphase boundaries between dots and the substrate [12-14]), composition and shape [1-9] of QDs, that affect the outstanding optoelectronic properties of such dots. This causes interest to analysis of defects and effective strains (associated with deviations of QDs from their equilibrium spatial positions) in QD arrays. Recently, such an analysis has

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

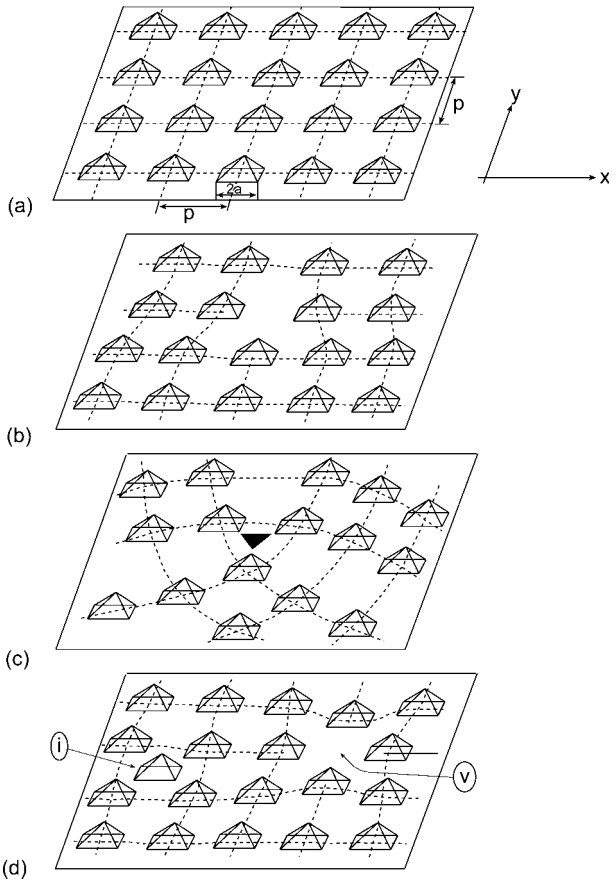

Fig. 1. States of 2D array consisting of free standing quantum dots on crystalline substrate. (a) Ideal (defect free) array. Array with (b) edge dislocation, (c) wedge disclination (triangle), and (d) vacancy and interstitial quantum dot.

been performed for the case of misfit dislocation lattices [20]. The main aim of this paper is to suggest a theoretical model which describes defects (Fig. 1 b, c and d) in QD arrays, with emphasis on their elastic and energetic characteristics.

2. ELASTIC CHARACTERISTICS OF STRAINED ARRAYS OF QUANTUM DOTS

Let us consider a model heteroepitaxial system consisting of an array of QDs and a thick substrate. In the framework of our model, QDs represent identical free standing pyramidlike nanoislands, each characterized by the base length 2*a* and the contact angle θ of its free surface with the substrate (Fig. 1). The nanoislands and the substrate are assumed to be isotropic solids having the same values of the shear modulus *G* and the same values of Poisson ratio ν. The geometric mismatch at the nanoisland/substrate boundaries is characterized by the misfit parameter $f=2(a_s-a_i)/(a_s+a_i)$, where a_i and a_s are the crystal lattice parameters of the nanoislands and the substrate, respectively. Following [17], the stresses induced by the nanoislands in the substrate due to the geometric mismatch at the nanoisland/substrate boundaries will be modeled here as quadrupoles of concentrated forces acting perpendicular to the substrate free surface. Owing to the quadrupole-quadrupole interaction associated with such stresses, neighbouring nanoislands (QDs) repel each other.

With the elastic interaction between QDs taken into account, one finds that they form a regular array whose symmetry depends on the orientation and elastic anisotropy of the substrate [15]. In this paper, for definiteness and simplicity, we restrict our consideration to square 2D arrays of QDs. The results of our consideration can be directly generalized to the situations with other symmetries of 2D arrays of QDs.

Let us examine elastic properties of a regular square ensemble of QDs with a period *p*. In the coordinate system shown in Fig. 1, the nodes of the ideal (non-strained) QD array (Fig. 1 a) have coordinates (x_k, y_l), where $x_k = kp$, $y_l = lp$, with *k* and *l* being integers. In order to describe effective elastic strains of the nanoisland array, we will model it as a two-dimensional elastic medium. In these circumstances, the displacements of QDs from array nodes are described by a two-dimensional vector displacement field $u_i(x,y)$. The corresponding effective strains of the nanoisland array are characterized by the strain tensor:

$$\varepsilon_{ij} = \frac{1}{2}(u_{i,j} + u_{j,i}), \quad i,j = x,y. \tag{1}$$

Let us represent the effective stresses in strained array of QDs as the sums of eigenstresses σ_{ij}^0 associated with repelling of QDs in non-strained array and "deviation" stresses σ_{ij} occurring due to deviations of QDs from their equilibrium spatial positions realized in the non-strained state of QD array. (The stresses σ_{ij}^0 occur as a result of the elastic interaction between QDs, which provides repulsion of QDs from each other. A balance between this interaction of the repulsion type and a release of the energy of the heteroepitaxial system due to nanoislanding determines the period *p* of the QD array.) In general, the stresses σ_{ij} are in a non-linear relationship with the strains ε_{mn}. For definiteness and simplicity, hereinafter we restrict our consideration to the situation with low strains ($\varepsilon_{mn}<<1$). In doing so, the linear dependence of the stress tensor $\boldsymbol{\sigma}$ on the strain tensor $\boldsymbol{\varepsilon}$ is realized with a good accuracy. It can be found as the first-order term of expansion of the tensor $\boldsymbol{\sigma}$ into power terms of $\boldsymbol{\varepsilon}$. In the discussed case of a square array of QDs, the three following elastic constants, c_{11}, c_{12} and c_{44}, figure in the linear relationship between components of the tensors σ_{ij} and ε_{ij}:

$$\sigma_{xx} = c_{11}\varepsilon_{xx} + c_{12}\varepsilon_{yy} + o(\varepsilon), \quad (2)$$

$$\sigma_{yy} = c_{11}\varepsilon_{yy} + c_{12}\varepsilon_{xx} + o(\varepsilon), \quad (3)$$

$$\sigma_{xy} = 2c_{44}\varepsilon_{xy} + o(\varepsilon). \quad (4)$$

Here c_{11}, c_{12} and c_{44} are the 2D elastic moduli whose units differ from those of bulk elastic moduli. From formulae (2)-(4) it follows that $c_{11}=\partial\sigma_{xx}/\partial\varepsilon_{xx}$ ($\boldsymbol{\varepsilon}$=0), $c_{12}=\partial\sigma_{xx}/\partial\varepsilon_{yy}$ ($\boldsymbol{\varepsilon}$=0), and $c_{44}=(1/2)\partial\sigma_{xy}/\partial\varepsilon_{xy}$ ($\boldsymbol{\varepsilon}$=0).

The elastic energy density (per unit substrate area) ω^{surf} that characterizes the strained array of QDs is defined as follows:

$$\omega^{surf} = \frac{1}{2}\left(\sigma_{ij}^{0} + \sigma_{ij}\right)\varepsilon_{ij}, \quad (5)$$

where the summation over repeated indices is performed. From (2)–(5), we get:

$$\frac{1}{2}\sigma_{ij}^{0} + \sigma_{ij} = \frac{\partial\omega^{surf}}{\partial\varepsilon_{ij}}, \quad (6)$$

$$\sigma_{ij}^{0} = 2\frac{\partial\omega^{surf}}{\partial\varepsilon_{ij}}(\boldsymbol{\varepsilon}=0), \quad (7)$$

and, as a corollary,

$$\sigma_{ij} = \frac{\partial\omega^{surf}}{\partial\varepsilon_{ij}}(\boldsymbol{\varepsilon}) - \frac{\partial\omega^{surf}}{\partial\varepsilon_{ij}}(\boldsymbol{\varepsilon}=0). \quad (8)$$

It should be noted that the stresses σ_{ij}^{0} and σ_{ij}, given by formulas (7) and (8), play the role of 2D stresses, and their units differ from those of bulk stresses.

Let us numerate nanoislands located in the ideal (non-deformed) state at array nodes having coordinates (x_k, y_l) by indices (k, l). Then the surface energy density ω^{surf} of the strained array of QDs can be re-written as:

$$\omega^{surf} = \frac{1}{2p^2}\sum_{\substack{i,j=-\infty \\ i^2+j^2\neq 0}}^{+\infty} W^{isl-isl}(r_{ij}), \quad (9)$$

where $W^{isl-isl}(r_{ij})$ denotes the energy that characterizes the elastic interaction between the (0, 0)– and (i, j)-nanoislands, and r_{ij} the distance between these nanoislands. In doing so, the energy $W^{isl-isl}(r)$ of the elastic interaction between two nanoislands distant by r from each other is calculated using the following general formula:

$$W^{isl-isl} = \frac{G\alpha V}{1-\nu}\Big[\left(\in_{rr}+f\right)^2 + 2\nu\left(\in_{rr}+f\right)\left(\in_{\varphi\varphi}+f\right) + \left(\in_{\varphi\varphi}+f\right)^2 - 2(1+\nu)f^2\Big]. \quad (10)$$

Here α (<1) denotes the factor taking into account stress relaxation in nanoislands, $\in_{rr}$ and $\in_{jj}$ are the strains induced by one nanoisland in the base center of another nanoisland. $V=(4/3)a^3\tan\theta$ is the pyramidlike nanoisland volume.

The strains $\in_{rr}$ and $\in_{jj}$ figuring in formula (10) are given as [17]:

$$\in_{rr} = \frac{Cf}{r^3}, \quad (11)$$

$$\in_{\varphi\varphi} = -\frac{Cf}{2r^3}, \quad (12)$$

where $C=(4\beta/\pi)\tan\theta\,(1+\nu)a^3$, and $\beta\approx 1$. With formulas (11) and (12) and the condition $C/r^3<<1$, formula (10) can be re-written in the following form:

$$W^{isl-isl} = \frac{M}{r^3}, \quad (13)$$

where

$$M = \frac{16\alpha\beta(1+\nu)^2}{3\pi(1-\nu)}f^2 G a^6\tan^2\theta. \quad (14)$$

In doing so, the term $a^6\tan^2\theta$, which is proportional to the product of two nanoisland volumes, appears in formula (14), because it characterizes the pair interaction between nanoislands, dependent on the volume of each nanoisland involved into the interaction.

In order to calculate the elastic moduli c_{11}, c_{12} and c_{44}, let us consider the QD array characterized by a spatially uniform strain $\varepsilon=\varepsilon_{xx}\boldsymbol{e}_x\boldsymbol{e}_x + \varepsilon_{yy}\boldsymbol{e}_y\boldsymbol{e}_y + \varepsilon_{xy}(\boldsymbol{e}_x\boldsymbol{e}_y + \boldsymbol{e}_y\boldsymbol{e}_x)$ (Fig. 2). In this situation, $r_{ij}=p[i^2(1+\varepsilon_{xx})^2+j^2(1+\varepsilon_{yy})^2+4ij\,\varepsilon_{xy}]^{1/2}$. Then, with formulas (9) and (13), we have:

$$\omega^{surf} = \frac{M}{2p^5}\sum_{\substack{i,j=-\infty \\ i^2+j^2\neq 0}}^{+\infty}\frac{1}{\left[i^2(1+\varepsilon_{xx})^2 + j^2(1+\varepsilon_{yy})^2 + 4ij\varepsilon_{xy}\right]^{3/2}}. \quad (15)$$

From formulas (7), (8) and (15), with the conditions that $c_{11}=\partial\sigma_{xx}/\partial\varepsilon_{xx}$ ($\boldsymbol{\varepsilon}$=0), $c_{12}=\partial\sigma_{xx}/\partial\varepsilon_{yy}$ ($\boldsymbol{\varepsilon}$=0) and $c_{44}=(1/2)\partial\sigma_{xy}/\partial\varepsilon_{xy}$ ($\boldsymbol{\varepsilon}$=0), we find:

$$\sigma_{xx}^{0} = \sigma_{yy}^{0} = \sigma^{0} = -\frac{3S_1M}{p^5}, \quad \sigma_{xy}^{0} = 0, \quad (16)$$

$$c_{11} = \frac{15S_2M}{2p^5}, \; c_{12} = \frac{15S_3M}{2p^5}, \; c_{44} = 2c_{12}, \quad (17)$$

where M is given by formula (14), and

$$S_1 = \sum_{\substack{i,j=-\infty \\ i^2+j^2\neq 0}}^{+\infty} \frac{i^2}{(i^2+j^2)^{5/2}} = 4.48,$$

$$S_2 = \sum_{\substack{i,j=-\infty \\ i^2+j^2\neq 0}}^{+\infty} \frac{i^2}{(i^2+j^2)^{7/2}} = 3.71, \qquad (18)$$

$$S_3 = \sum_{\substack{i,j=-\infty \\ i^2+j^2\neq 0}}^{+\infty} \frac{i^2 j^2}{(i^2+j^2)^{7/2}} = 0.76.$$

3. DISLOCATIONS, DISCLINATIONS AND POINT DEFECTS IN QUANTUM DOT ARRAYS

Let us examine energetic characteristics of defects (Fig. 1 b, c and d) in 2D arrays of QDs, using c_{11} and c_{12} calculated. In doing so, in our approximation treating the QD array as an elastically isotropic system, its elastic properties are characterized by the averaged shear modulus $\overline{G}_i$ and Poisson ratio $\overline{\nu}_i$. Formulas (2)-(4) and the following 2D analog of Hooke's law:

$$\sigma_{ij} = \frac{2\overline{G}_i}{1-\overline{\nu}_i}\left[(1-\overline{\nu}_i)\varepsilon_{ij} + \overline{\nu}_i \varepsilon_{kk}\delta_{ij}\right] \qquad (19)$$

(where $i,j=x,y$; $\varepsilon_{kk}=\varepsilon_{xx}+\varepsilon_{yy}$, and δ_{ij} is the Kronecker symbol) result in the following expressions: $\overline{\nu}_i = c_{12}/c_{11} \approx 0.2$ and $\overline{G}_i = \gamma(c_{11}-c_{12})/2 \approx 0.4\,\gamma\, c_{11}$. Here γ is the factor taking into account anisotropy ($\gamma \sim 1$). It should be noted that equation (19) formally coincides with Hooke's law for a 3D medium in the plane stress state.

The energy of a defect in a QD array, by analogy with the energy of a defect in conventional crystal lattice, is defined as the difference between energies of this QD array with and without the defect. In order to calculate the energy of a defect, it is necessary to rigorously define the transformation of QD array from its initial non-defected state into a defected state. In the situation with a conventional crystal lattice, a transformation from a non-defected state into a defected state is associated with addition of extra atoms to the lattice or removal of atoms from the lattice, with consequent elastic relaxation [21]. The transformation discussed does not lead to a dramatic change of the atomic density, because elastic relaxation is caused by a balance between interatomic interactions of both repulsion and attraction types. The attraction-type interaction is absent in QD arrays, in which case the interspacing between QDs is determined by a balance between their elastic interaction of the only repulsion type and the nanoislanding. A detailed analysis of the balance is beyond the scope of this paper focusing on elastic properties of QD arrays. Therefore, for definiteness, hereinafter, we assume that transformations from the non-defected state (Fig. 1 a) of a 2D array of QDs to its defected states (Fig. 1 b,c and d) occur with the proviso that the mean density of QDs is the same in the non-defected and defected states.

With the above assumption, the transformation can be treated as the following imaginary two-step procedure. At the first step, a 2D array consisting of N QDs is uniformly strained, in which case the mean density of QDs changes by factor $(N+u\,n)/N$, where n is an integer, and $u=\pm 1$. That is, the QD array undergoes uniform compressive or tensile deformation. At the second step (which is identical to conventional transformation of non-defected crystal lattice to defected one [21]), a defect is introduced into the uniformly strained QD array by removing (if $u=1$) n QDs from the array or adding (if $u=-1$) n extra QDs to the array, with consequent elastic relaxation of the defected array of QDs. n and the sign of u depend on the type of defect. The mean density of QDs is the same before and after the two-step transformation.

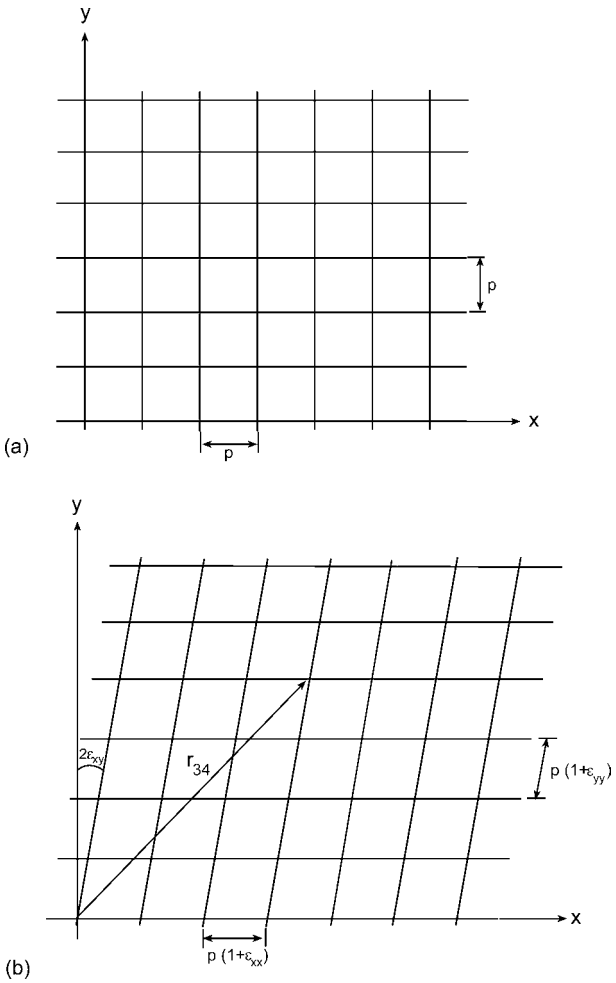

Fig. 2. (a) Non-strained and (b) uniformly strained arrays of quantum dots.

As a result of the first step of the transformation discussed, the QD array is still non-defected and strictly periodic, but its period changes by the factor $\sqrt{N/(N+un)}$, giving rise to the following change W_l of the elastic energy of the QD array:

$$W_l = \lim_{N\to\infty}\left[W_0\left(p\sqrt{\frac{N}{N+un}}\right) - W_0(p)\right]. \qquad (20)$$

Here $W_0(t)$ is the sum energy that characterizes elastic interaction between QDs forming the square-lattice-type array with period t. It is calculated using formula:

$$W_0(t) = \frac{N}{2}\sum_{\substack{i,j=-\infty \\ i^2+j^2\neq 0}}^{+\infty} W^{isl-isl}(t\sqrt{i^2+j^2}). \qquad (21)$$

Substitution of (13) and (21) into formula (20) gives:

$$W_l = \frac{3unMS_4}{4p^3}. \qquad (22)$$

Here $S_4 = \sum_{\substack{i,j=-\infty \\ i^2+j^2\neq 0}}^{+\infty} \frac{1}{(i^2+j^2)^{3/2}} = 8.96.$

The QD array with a defect (e.g., dislocation, disclination, vacancy, interstitial QD), resulting from the second step of the transformation from a non-defected state to a defected state, is characterized by the energy density (per unit area) w^{surf} defined by formula (5). This energy density can be represented as the sum of the proper elastic energy (self-energy) density $(1/2)\sigma_{ij}\varepsilon_{ij}$ of the defect and the energy density $(1/2)\sigma^0_{ij}\sigma_{ij}$ of the interaction between the defect and the stress field $\boldsymbol{\sigma}^0$ acting in the non-strained state of the QD array due to QD repulsion.

The self-energy W^d_{self} of an edge dislocation (Fig. 1 b) in the center of a QD array (where the plane stress state is realized) occupied the surface of a circle of radius R is given by the formula similar to the general expression [21] for the elastic energy of an edge dislocation in a three-dimensional lattice, with ν_i replaced by $\nu_i/(1+\nu_i)$ [22]. In doing so, we get:

$$W^d_{self} = \frac{D'p^2}{2}\left(\ln\frac{R}{p} + Z\right). \qquad (23)$$

Here $D'=G_i(1+\nu_i)/(2\pi)$, p plays the role of the dislocation Burgers vector modulus (equal to period of the QD array), and Z ($\approx$1) denotes the factor taking into account the contribution of the dislocation core to the energy W^d_{self}.

As with conventional dislocations in real crystals [23], the energy W^d_{int} that characterizes interaction between the dislocation and the stress field $\boldsymbol{\sigma}^0$ is calculated using formula:

$$W^d_{int} = pu\sigma^0 R. \qquad (24)$$

The total energy W^d of the dislocation being equal to the sum $W^d_{self}+W^d_{int}+W_l$ is derived from formulas (16), (18), (22)-(24) and the condition $n=R/p$ as follows:

$$W^d = \frac{D'p^2}{2}\left(\ln\frac{R}{p} + Z - 6.3\frac{u}{\gamma}\frac{R}{p}\right). \qquad (25)$$

Similar to dislocations (see above), the energy W^Δ of a wedge disclination in a 2D array of QDs (Fig.1c) is represented as the sum $W^\Delta_{self}+W^\Delta_{int}+W_l$, where W^Δ_{self} denotes the proper energy of the disclination, W^Δ_{int} the energy that characterizes interaction of the disclination and the stress field $\boldsymbol{\sigma}^0$, and W_l the energy that characterizes uniform strains due to the first (imaginary) step of the formation of the defect.

Following the general theory of disclinations in solids [24], the self-energy of an isolated wedge disclination of strength ω, located in the center of QD array occupying a disc-like free surface of the substrate of radius R, is given as:

$$W^\Delta = \frac{D'\omega^2R^2}{8}. \qquad (26)$$

The energy W^Δ_{int} that characterizes interaction between the disclination and the stress field $\boldsymbol{\sigma}^0$ is calculated using formula [23]:

$$W^\Delta_{int} = -\frac{\omega\sigma^0R^2}{2}. \qquad (27)$$

Here the disclination strength $\omega > 0$ ($\omega < 0$, respectively), if the disclination formation is associated with addition of extra QDs (removal of QDs, respectively) at the second stage.

From formulas (16)-(18), (22), (26) and (27) and the condition $n=-\omega R^2/(2up^2)$, we find the total energy W^Δ of the disclination in the QD array to be:

$$W^\Delta = \frac{D'\omega R^2}{8}\left(\omega + \frac{12.6}{\gamma}\right). \qquad (28)$$

Since $W^\Delta \propto R^2$, the formation of isolated disclinations (Fig. 1 c) is highly unfavourable in real QD systems. In general, however, as with conventional disclinations in solids (e.g., [24-28]), disclinations in QD array can form configurations with screened stress fields. In this case they can exist as (quasi)stable defects in QD arrays.

In spirit of conventional models [21] treating point defects in three-dimensional solids as elastic balls with extra or deficient free volume in three-dimen-

sional elastic media, we will model elastic relaxation of QD ensembles with point defects (Fig. 1 d) as being induced by inserting elastic disks into initially empty disc-like regions in thin plate. (Here and in the following, we restrict the term "point defect" to vacancies and interstitial QDs, although dislocations and disclinations in a two-dimensional QD array can be considered as point defects as well). In doing so, vacancies and interstitial QDs are characterized by respectively negative and positive difference Δr between the radii $r_0+\Delta r$ and r_0 of the inserted disc and empty disc-like region. In the framework of the model discussed, the self-energy W_{self} of a point defect can be written as follows:

$$W_{self}^{p} = 2\pi\overline{G}_i(\Delta r)^2. \qquad (29)$$

The energy W_{int}^{p} that characterizes the interaction of a point defect with the stress field σ^0 can be calculated [23] as

$$W_{int}^{p} = \frac{\pi\eta\overline{G}_i r_0 \Delta r}{\gamma}, \qquad (30)$$

where $\eta = |\gamma\sigma^0/\overline{G}_i|=1.21$.

In the case of vacancies and interstitial QDs, with formulas (22), (29) and (30), we have the total energy $W^p = W_{self}^{p}+W_{int}^{p}+W_l$ (n=1) of a vacancy or an interstitial QD to be given as:

$$W^p = \overline{G}_i p^2\left[2\pi\left(\frac{\Delta r^2}{p}\right) - \pi\eta u\frac{r_0|\Delta r|}{\gamma p^2} + \frac{uS_4}{4\gamma S_2}\right]. \qquad (31)$$

Dependences $W^p(|\Delta r/p|)$, for a vacancy (with $r_0=p$ and $u=1$) and interstitial QD (with $r_0=p/\sqrt{2}$ and $u=-1$) are shown in Fig. 3 for the case $\gamma=1$. From Fig. 3 it follows that the energy of a vacancy with $|\Delta r|=(0.2\text{-}0.4)\,p$ is in the range of $W^p=(0.35\text{-}0.5)\overline{G}_i p^2$. The energy of an interstitial QD strongly depends on Δr. For $\Delta r/p=(0.2\text{-}0.4)$, it is in the range of $W^p=(0.2\text{-}1.5)\,\overline{G}_l p^2$.

It should be noted that the energy of a vacancy in 2D array of QDs is close to the energy of a conventional vacancy in real crystals. Actually, the elastic energy W_{3D}^{p} of a point defect in a crystal, modeled as an elastic ball with radius $\tilde{r}_0+\Delta\tilde{r}$, inserted into a ball-like pore with radius r_0, is as follows: $W_{3D}^{p}=8\pi G\, r\,(\Delta r)^2$. For characteristic values of $\tilde{r}_0=b$, $\Delta\tilde{r}=-0.2\,b$, $p=100\,b$ (with b being the interatomic distance in a crystal), $r_0=-0.2\,p$, $\theta=11°$ and $2a/p=0.4\text{-}0.8$, we have: $W^p/W_{3D}^{p}=0.04\text{-}2.5$. A similar situation is with interstitial QDs in QD arrays and interstitial atoms in real crystals. As a corollary, similar to conventional point defects in real crystals, vacancies and interstitial QDs can be intensively formed in QD arrays fabricated at non-equilibrium conditions.

Following experimental data [16, 29, 30], large dome-like QDs are formed in arrays of small pyramidal QDs. Their formation breaks uniformity of QDs in size and shape, leading to degradation of their functional properties [16, 29, 30]. Recently, Ref. [8] has reported on experimental observation of the formation of small pyramidal QDs in arrays of large dome-like QDs. In terms of point defects, minority QDs (dome-like QDs in arrays of pyramidal QDs and pyramidal QDs in arrays of dome-like QDs) can be treated as impurity-like defects. In the first approximation such defects are described as point dilatation centers with positive or negative dilatation, depending on their size. The elastic energy of an impurity-like defect is equal to the sum $W_{self}^{p}+W_{int}^{p}$. It should be taken into account in analysis of experimentally detected [16, 29, 30] shape transformations of QDs.

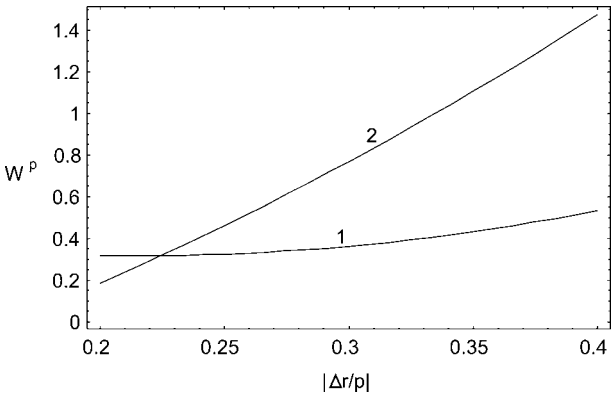

Fig. 3. Dependences of energy W^p (in units $\overline{G}_l p^2$) of vacancy (curve 1) and interstitial quantum dot (curve 2) in 2D array of quantum dots on parameter $|\Delta r/p|$, for $\gamma = 1$.

4. CONCLUDING REMARKS

Thus, in this paper, we have theoretically examined QD ensembles of the new type – the QD arrays with defects (Fig. 1 b, c and d) – with focuses placed on their elastic characteristics, such as elastic moduli and elastic energies of defects. It is shown that vacancies and interstitial QDs (Fig. 1 d) are characterized by energies whose values are close to those of conventional point defects in real crystals. As a corollary, vacancies and interstitial QDs, similar to their counterparts in real crystals, can be intensively formed in QD arrays fabricated at highly non-equilibrium conditions (which are rather conventional in real technologies). Defects (Fig. 1 b, c and d) cause irregularities in spatial arrangement of QDs and, therefore, the conventional stress distribution in QD/substrate composite, which, in its turn, strongly affects diffusion, Ostwald ripening, conventional misfit (lattice) dislocation formation and shape transformations in

QDs. The processes discussed strongly influence the outstanding functional properties of QD ensembles. In this context, of special importance will be experimental identification of the structural and behavioral features of QD arrays containing defects (Fig. 1 b, c, and d). These features should be definitely taken into consideration in further experimental and theoretical study of QD ensembles, because of their fundamental significance and potential use in technological applications. The results of the theoretical analysis of this paper can be used also in studies of ordered ensembles of vortices in superconductors, superfluids, ferromagnetic materials, etc.

ACKNOWLEDGEMENTS

This work was supported, in part, by the Office of US Naval Research (grant N00014-01-1-1020), the Office of US Naval Research, International Field Office, Europe (grant N00014-02-1-4045), NATO Science Programme (grant PST.CLG.977712), the Russian Fund of Basic Researches (grant 01-02-16853), Integration Program (grant B0026) and St. Petersburg Scientific Center of Russian Academy of Sciences.

REFERENCES

[1] V.A. Shchukin and D. Bimberg // *Rev. Mod. Phys.* **71** (1999) 1125.
[2] J.A. Floro, M.B. Sinclair, E. Chanson, L.B. Freund, R.D. Twesten, R.Q. Hwang and G.A. Lucadamo // *Phys. Rev. Lett.* **84** (2000) 701.
[3] W.V. Schoenfeld, C. Metzner, E. Letts and P.M. Petroff // *Phys. Rev. B* **63** (2001) 205319.
[4] I. Kegel, T.H. Metzger, A. Lorke, J. Peisl, J. Stangl, G. Bauer, K. Nordlund, W.V. Schoenfeld and P.M. Petroff // *Phys. Rev. B* **63** (2001) 035318.
[5] P.B. Joyce, T.J. Krzyzewski, G.R. Bell, A. Joyce and T.S. Jones // *Phys. Rev. B* **58** (1998) R15981.
[6] N. Liu, J. Tersoff, O. Baklenov, A.L. Holmes, Jr. and C.K. Shih // *Phys. Rev. Lett.* **84** (2000) 334.
[7] T. Walter, A.G. Cullis, D.J. Norris and M. Hopkinson // *Phys. Rev. Lett.* **86** (2001) 2381.
[8] A. Rastelli, M. Kummer, and H. von Kaanel // *Phys. Rev. Lett.* **87** (2001) 256101.
[9] S.A. Chaparro, Y. Zhang, J. Drucker, and D.J. Smith // *J. Appl. Phys.* **87** (2000) 2245.
[10] S.A. Chaparro, J. Drucker, Y. Zhang, D. Chandrasekhar, M.R. McCartney, D.J. Smith // *Phys. Rev. Lett.* **83** (1999) 1199.
[11] J. Seufert, G. Bacher, M. Scheibner, A. Forchel, S. Lee, M. Dobrowolska, and J.K. Furdina // *Phys. Rev. Lett.* **88** (2002) 027402.
[12] H.T. Johnson and L.B. Freund // *J. Appl. Phys.* **81** (1997) 6081.
[13] R.V. Kukta and L.B. Freund // *J. Mech. Phys. Solids* **45** (1997) 1835.
[14] I.A. Ovid'ko // *Phys. Rev. Lett.* **88** (2002) 046103.
[15] V. Holy, G. Springholz, M. Pinczolits and G.Bauer // *Phys. Rev. Lett.* **83** (1999) 356.
[16] B. Voigtländer and N. Theuerkauf // *Surf. Sci.* **461** (2000) L575.
[17] I.A. Ovid'ko and A.G. Sheinerman // *Appl. Phys. A* **74** (2992) 273.
[18] A. Bouret // *Surf. Sci.* **432** (1999) 37.
[19] G. Medeiros-Ribeiro, T.I. Kamins, D.A.A. Ohlberg and R.S. Williams // *Phys. Rev. B* **58** (1998) 3533.
[20] I.A. Ovid'ko and A.G. Sheinerman // *J. Phys.: Condens. Matter* **15** (2003) 2127.
[21] J.P. Hirth and J. Lothe, *Theory of Dislocations* (John Wiley, New York, 1982).
[22] S.P. Timoshenko and J.N. Goodier, *Theory of Elasticity* (McGraw-Hill, New York, 1970).
[23] T. Mura, In: Advances in Materials Research, Vol. 3, ed. by H. Herman (Interscience Publishers, New York, 1968), p. 1.
[24] A.E. Romanov and V.I. Vladimirov, *Dislocations in Solids*, Vol. 9, ed. by F.R.N. Nabarro (North-Holland Publ. Co., Amsterdam, 1992), p. 191.
[25] A.A. Nazarov, A.E. Romanov and R.Z. Valiev // *Acta Metall. Mater.* **41** (1993) 1033.
[26] S.V. Bobylev, I.A. Ovid'ko and A.G. Sheinerman // *Phys. Rev. B* **64** (2001) 224507.
[27] I.A. Ovid'ko // *Science* **295** (2002) 2386.
[28] M. Murayama, J.M. Howe, H. Hidaka and S. Takaki // *Science* **295** (2002) 2433.
[29] G. Medeiros-Ribeiro, A.M. Bratkovski, T.I. Kamins, D.A.A. Ohlberg and R.S. Williams // *Science* **279** (1998) 353.
[30] F.M. Ross, R.M. Tromp and M.C. Reuter // *Science* **286** (1999) 1931.