SOME THERMODYNAMIC ASPECTS OF SELF-ASSEMBLY OF ARRAYS OF QUANTUM DOTS

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Abstract. We have studied the relative adhesion (the wetting) of dislocation-free three-dimensional islands belonging to an array of islands to the wetting layer in Stranski-Krastanov growth mode. The array has been simulated as a chain of islands in 1+1 dimensions placed on top of a wetting layer. In addition to the critical size of the two-dimensional islands for the 2D-3D transformation to occur, we find that the wetting depends strongly on the density of the array, the size distribution and the shape of the islands.

1. Introduction

The instability of planar films against coherently strained three-dimensional (3D) islands in highly mismatched epitaxy is a subject of intense research in recent time owing to their possible optoelectronic applications as quantum dots.[1] The term “coherent Stranski-Krastanov (SK) growth” has been coined for this case of formation of 3D islands that are strained to fit the underlying wetting layer at the interface but are largely strain-free near their top and side walls.[2, 3] This term was introduced in order to distinguish this case from the “classical” SK growth in which the lattice misfit is accommodated by misfit dislocations at the interface.[4]

Experimental studies of arrays of coherent 3D islands in SK growth of highly mismatched semiconductor materials one on top of the other have
shown surprisingly narrow size distributions of the islands,[5, 6, 7, 8] (see also Ref. [3] and the references therein). (It is worth noting that a narrow size distribution has been established also in the Volmer-Weber growth of metals on insulators in the absence of a wetting layer.[9]) This phenomenon, known in the literature as self-assembly (for a review see Ref. [10]), is highly desirable as it guarantees a specific optical wavelength of the array of quantum dots. The physics of this self-assembly is still not understood in spite of the numerous thermodynamic and kinetic studies.[11, 12, 13, 14] For example, Priester and Lannoo found that two-dimensional (2D) islands with a monolayer height act as precursors of the 3D pyramidal islands,[15] (see also Ref. [16]). The energy per atom of the 2D islands possesses a minimum for a certain volume, but the 3D islands become energetically favored at a smaller size. Thus, at some critical surface coverage, the 2D islands spontaneously transform into 3D islands preserving a nearly constant volume during the 2D-3D transformation. The resulting size distribution reflects that of the 2D islands which is very narrow. This picture has been recently corroborated by Ebiko et al.[17] who found that the volume distribution of InAs/GaAs self-assembled quantum dots agrees well with the scaling function that is characteristic for the two-dimensional submonolayer homoepitaxy. [18] Korutcheva et al.[19] and Markov and Prieto [20] reached the same conclusion with the exception that the 2D-3D transformation was found to take place through a series of intermediate states with discretely increasing thickness (one, two, three, etc. monolayers-thick islands) that are stable in separate consecutive intervals of volume. Khor and Das Sarma arrived to the same conclusion by using Monte Carlo simulations.[21]

In a recent paper, Prieto and Markov discussed the formation of coherent 3D islands within the framework of the traditional concept of wetting.[22] As is well known the wetting parameter which accounts for the energetic influence of a crystal B in the heteroepitaxial growth of a crystal A on top of it is defined as (for a review see Ref. [23])

$$\Phi = 1 - \frac{E_{AB}}{E_{AA}}$$

where $E_{AA}$ and $E_{AB}$ are the energies per atom required to disjoin a half-crystal A from a like half-crystal A and from an unlike half-crystal B, respectively.

The mode of growth of a thin film is determined by the difference $\Delta \mu = \mu(n) - \mu_{3D}^0$, where $\mu(n)$ and $\mu_{3D}^0$ are the chemical potentials of the film (as a function of its thickness $n$) and of the bulk material A, respectively.[23] The chemical potential of the bulk crystal A is given at zero temperature by the work $\phi_{AA}$ (taken with a negative sign) to detach an atom from the well known kink or half-crystal position. The latter name is due to the fact
that an atom at this position is bound to a half-atomic row, a half-crystal plane and a half-crystal block.[24, 25] In the case of a monolayer-thick film of A on the surface of B the chemical potential of A is given by the analogous work $\phi_{AB}$ with the exception that the underlying half-crystal block of A is replaced by a half-crystal block of B. Thus $\Delta \mu = \phi_{AA} - \phi_{AB}$. In the simplest case of additivity of bond energies the difference $\phi_{AA} - \phi_{AB}$ reduces to $E_{AA} - E_{AB}$ as the lateral bondings cancel each other. Then $\Delta \mu$ is proportional to $\Phi$, i.e. $\Delta \mu = E_{AA}\Phi$. It follows that it is the wetting parameter $\Phi$ which determines the mechanism of growth of A on B.[26] In the two limiting cases of growth of isolated 3D islands of A directly on the surface of B [Volmer-Weber growth, characterized by incomplete wetting ($0 < \Phi < 1$) and any misfit $\varepsilon_0 = \Delta a/a$, or by consecutive formation of monolayers of A on B [Frank- van der Merwe growth, with complete wetting ($\Phi \leq 0$) and $\varepsilon_0 \approx 0$], $\Delta \mu$ goes asymptotically to zero from above and from below, respectively, but it changes sign in the case of growth of 3D islands of A on a thin wetting layer of A on the substrate B [Stranski-Krastanov growth, complete wetting at the beginning ($\Phi \leq 0$) and $\varepsilon_0 \neq 0$].[22, 23] Equation $\Delta \mu = E_{AA}\Phi$ is thus equivalent to the familiar 3-$\sigma$ criterion of Bauer.[23, 27]

The Stranski-Krastanov morphology appears as a result of the interplay of the film-substrate bonding, misfit strain and the surface energies. A wetting layer with a thickness of the order of the range of the interatomic forces is first formed (owing to the interplay of the A-B interaction and the strain energy accumulation) on top of which partially or completely relaxed 3D islands nucleate and grow. The 3D islands and the thermodynamically stable wetting layer represent necessarily different phases. If this were not the case, the growth would continue by 2D layers. Thus we can consider as a useful approximation to regard the 3D islanding on top of the uniformly strained wetting layer as a Volmer-Weber growth. That requires the mean adhesion of the atoms that belong to the base plane of the 3D islands to the stable wetting layer to be smaller than the cohesion between them. In other words, the wetting of the underlying wetting layer by the 3D islands must be incomplete. Otherwise, 3D islanding will not occur.[26] In the Volmer-Weber growth the incomplete wetting is due mainly to the difference in bonding ($E_{AB} < E_{AA}$), the supplementary effect of the lattice misfit being usually smaller. In the coherent SK growth ($E_{AB} \approx E_{AA}$), the incomplete wetting is due to the lattice misfit, which leads to the atoms at the edges of the islands to displace from the bottoms of the potential troughs provided by the atoms in the layer underneath.[28, 22]

As has been shown elsewhere,[19, 22] it is the incomplete wetting which determines the formation of dislocation-free 3D islands on top of the wetting layer in the case of coherent SK growth. In this case, however, the relation
between $\Delta \mu$ and $\Phi$ is not as simple as given above. The bond energies are generally not additive, the misfit strain is relaxed mostly near the side and top walls and increasing the island’s thickness leads to larger displacements of the edge atoms from the bottoms of the potential troughs provided by the wetting layer and in turn to a decrease of the wetting. For this reason, in this work we define the wetting parameter $\Phi$ as the difference of the interaction energies with the wetting layer of misfitting and non-misfitting 3D islands.

In the present paper we study the behavior of $\Phi$ for islands which belong to an array of islands. We study the effect of the density of the array (the distance to the nearest neighbor islands), the size distribution (the difference in size of the neighboring islands), and the shape distribution (the slope of the side walls of the neighboring islands) on the wetting parameter $\Phi$ of the considered island.

2. Model

We consider an atomistic model in $1+1$ dimensions (lateral size + height) which we treat as a cross section of the real $2+1$ dimensional case. An implicit assumption is that in the real $2+1$ dimensional model the monolayer islands have a compact rather than a fractal shape and that the lattice misfit is the same in both orthogonal directions. The 3D islands are represented by linear chains of atoms stacked one upon the other.[29, 30] Each upper chain is shorter than the lower one. The shape of the islands in our model is given by the slope of the side walls. For, example, an island which consists of consecutive chains with $N$, $N-1$, $N-2$... atoms has a $60^\circ$ slope of the side walls, whereas an island with chains consisting of, say, $N$, $N-5$, $N-10$... atoms has a slope of $19.1^\circ$, etc., where $N$ is the number of atoms in the base chain. The array in the 1+1 dimensional space is represented by a row of 3 or 5 islands on a wetting layer consisting of several monolayers (Fig. 1). The distance between two neighboring islands is given by the number $n$ of vacant atomic positions between the ends of their base chains and can be varied from one to infinity.

Figure 1. Schematic view of an array of islands on a wetting layer. The central island is surrounded by two islands with different shapes and sizes. By $n$ is denoted the spacing between neighboring islands, which is a measure of the density of the array.
In order to simplify the computational procedure the “wetting layer” in our model is in fact composed of several monolayers of the true wetting layer consisting of atoms of the overlayer material A plus several monolayers of the unlike substrate material B. This composite wetting layer has the atom spacing of the substrate material B as in the real case, but for the sake of simplicity the atom bonding is that of the overlayer material A. We believe that the latter does not introduce a perceptible error as the energetic influence of the substrate B is screened by the true wetting layer A. We expect that this approximation underestimates to some extent the wetting parameter Φ by making the composite substrate a bit softer than the real one (the A-A bonding is weaker than the B-B bonding,[31] for a later review see Ref. [23]). We found that beyond 10 monolayers the studied parameter Φ saturates its value. This is why in all cases given below, unless otherwise stated, we allowed 10 monolayers to relax.

As in our previous work (Ref. [20]), we make use of a simple minimization procedure. The atoms interact through a potential that can be easily generalized to vary its anharmonicity by adjusting two constants μ and ν (μ > ν) that govern separately the repulsive and attractive branches, respectively,[32]

\[ V(x) = V_o \left[ \frac{\nu}{\mu - \nu} e^{-\mu(x-b)} - \frac{\mu}{\mu - \nu} e^{-\nu(x-b)} \right] , \]  

where \( b \) is the equilibrium atom separation. In this work, we have used \( \mu = 2\nu \) with \( \nu = 6 \), which turns the potential (2) into the familiar Morse form.

Our program calculates the interaction energy of all the atoms as well as its gradient with respect to the atomic coordinates, i.e. the forces. Atoms in the islands and in the wetting layer are then allowed to relax. Relaxation of the system is performed by allowing the atoms to displace in the direction of the gradient in an iterative procedure until the forces fall below some negligible cutoff value. Periodic boundary conditions are applied in the lateral direction. We consider only interactions in the first coordination sphere in order to mimic the directional bonds that are characteristic for most semiconductor materials.[33]

3. Results

Figure 2(a) shows the horizontal displacements of the atoms of the base chain from the bottoms of the potential troughs provided by the homogeneously strained wetting layer for a misfit of 7%. The considered island has two identical ones at a distance of \( n = 5 \). This is the same behavior as predicted by the one-dimensional model of Frank and van der Merwe.[28] The
horizontal displacements increase with increasing island thickness (measured in number of monolayers) precisely as in the case of a rigid substrate and non-interacting islands.[20] In contrast to the rigid substrate case,[22] the vertical displacements of the edge atoms of the base chain of the islands and the underlying atoms of the uppermost monolayer of the wetting layer are directed downwards (Fig. 2(b)). It is worth noting that the same result has been found by Lysenko et al. in the case of homoepitaxial metal growth by using a computational method within the framework of the tight-binding model.[34]

Figure 2. Horizontal (a) and vertical (b) displacements of the atoms of the base chain from the bottoms of the potential troughs provided by the homogeneously strained wetting layer, for a lattice misfit of 7%. The considered island has 16 atoms in the base chain and is located between two identical ones at a distance of \( n = 5 \). The displacements are given in units of the lattice parameter \( a \) of the composite wetting layer. The horizontal displacements increase with increasing island thickness taken in number of monolayers. Contrary to the rigid substrate case, the vertical displacements of the edge atoms of the base chain of the islands and those of the underlying atoms of the uppermost monolayer of the wetting layer, included in (b), are directed downwards.

In spite of their downwards vertical displacements, the edge atoms are again more weakly bound to the underlying wetting layer, as in the rigid
substrate models of Refs. [19] and [20] (Fig. 3). Shown in the same figure for comparison is also an island without neighbors. As seen, the edge atoms of the single island adhere more strongly to the substrate. This is in fact the essential physics behind the effect that the neighboring islands exert on the middle island. The central island loses to some degree contact with the substrate (in this case the wetting layer) and the wetting parameter is increased. We can interpret this as the wetting layer becoming stiffer under the influence of the neighboring islands.

The influence of the density of the array is demonstrated in Fig. 4. The values for 3 and 5 islands were calculated assuming equally spaced islands. These can be thus treated as a self-organized array. As expected the wetting parameter increases with decreasing distance between the islands or, in other words, with increasing array density.

Figure 5 shows the wetting parameter of the central island as a function of the size of the side islands. For this calculation, we considered three islands with the same thickness of 3 monolayers. Furthermore, both side islands have one and the same volume. Increasing the volume of the side islands leads to an increase of the elastic fields around them and to a further reduction of the bonding between the edge atoms of the central island and the wetting layer.

Figure 6 demonstrates one of the most important results, the effect of the size distribution on the wetting of the islands. It shows the behavior of the wetting parameter $\Phi$ of the central island as a function of the number
Figure 4. Dependence of the wetting parameter of the central island on the distance $n$ between the islands. Results for arrays of 3 and 5 islands are given, as well as for a reference isolated island. All islands are 3 ML-high, have 20 atoms in their base chains and the lattice misfit amounts to 7%. As seen, the next-nearest neighbors play a smaller but not negligible role.

Figure 5. Dependence of the wetting parameter of the central island on the size of the base chains of the two side islands. These two have the same volume and are separated from the central one by a distance $n = 5$. All the islands are 3 ML high, the central one having 20 atoms in the base chain, the misfit amounts to 7% and the wetting layer consists of 3 ML which are allowed to relax.

of atoms in the base chain (which is a measure of the volume) of the left island. In this case, the sum of the volumes (the total number of atoms) of the left and right islands is kept constant and precisely equal to the doubled volume of the central island. All three islands have the same thickness. The
Figure 6. Dependence of the wetting parameter of the central island on the size distribution of the side islands. The central island is three monolayers thick and has 20 atoms in the base chain thus containing a total of 57 atoms. The lattice misfit is 7%. The x-axis represents the number of atoms in the base chain of the left island. The sum of the volumes of the left and right islands is kept constant and equal to the doubled volume of the central island. We increase the volume of the left island and decrease the volume of the right island thus passing through the middle point at the maximum where the three islands have equal volumes.

Figure 7. Dependence of the wetting parameter of the central island on the shape of the neighboring islands, measured in degrees of their facet angles. The central island has a slope of 60° of its side walls. All islands are 3 ML high, have 20 atoms in their base chains and are separated by a distance $n = 5$. The lattice misfit amounts to 7%.

side walls of all the three islands make an angle of 60° with their bases. Thus the first point (and, by symmetry, also the last one) gives the maximum
asymmetry in the size distribution of the array, the left island consists of 9 atoms whereas the right island is built of 105 atoms. The point at the maximum of wetting describes the monodisperse distribution – the three islands have one and the same volume of 57 atoms. As seen in the case of perfect self-assembly of the array the wetting parameter, or in other words, the tendency to clustering displays a maximum value.

The effect of the shape of the side islands, i.e. their facet angles, on the wetting parameter of the central island is demonstrated in Fig. 7. The slope of the facets of the central island is 60°. The effect is greatest when the side islands have the steepest walls. The same result (not shown) is obtained when the central island has a different facet angle, e.g. 11°. The explanation follows the same line as the one given above. The side islands with larger-angle side walls exert a greater elastic effect on the wetting layer and in turn on the displacements and the bonding of the edge atoms of the central island.

![Figure 8](image)

*Figure 8.* Dependence of the energy per atom on the total number of atoms in compressed coherently strained islands with different thicknesses in monolayers denoted by the figures at each curve for a misfit of 7%. The considered island has two identical neighbours at a distance \( n = 5 \). The analogous curves for single isolated islands (empty symbols) are also given for comparison. The wetting layer consists in all cases of 3 ML which are allowed to relax.

We studied also the stability of islands with a thickness increasing by one monolayer in the presence of two islands on both sides on a deformable substrate. The result in Fig. 8 shows the same behavior observed in Refs. [19] and [20] where rigid substrates were assumed. This means that the overall transformation from the precursor 2D islands to a macroscopic 3D islands takes place in consecutive stages in each of which the islands thicken by one monolayer. As shown in Refs. [19] and [20] the latter leads in turn
to a critical misfit beyond which coherent 3D islanding takes place, and below which the lattice mismatch is accommodated by misfit dislocations. The existence of a critical misfit has been experimentally observed in a series of different systems,[5, 35, 36, 37] The energies computed in the case of the reference single islands always lie below the curves of the islands in an array. The difference obviously gives the energy of repulsion between the neighboring islands. It follows from the above that the presence of neighboring islands leads to a slight decrease of the critical misfit.

4. Discussion

For the discussion of the above results we have to bear in mind that a positive wetting parameter shows in fact a tendency of the deposit to form 3D clusters rather than a planar film. In the case of coherent SK growth, the non-zero wetting parameter is due to the weaker adhesion of the atoms that are closer to the islands edges. The presence of other islands, particularly with large angle facets, in the near vicinity of the considered island makes this effect stronger as seen in Fig. 3. The transformation of two-dimensional islands with a monolayer height into bilayer three-dimensional islands takes place by detachment of atoms from the edges and their subsequent jumping and collision on the top island’s surface.[38] Thus this edge effect clearly demonstrates the influence of the lattice misfit on the rate of second layer nucleation and in turn on the kinetics of the 2D-3D transformation.[39, 40] The presence of neighboring islands facilitates and thus accelerates the formation of 3D clusters and their further growth. In a self-assembled population of islands the tendency to clustering is thus enhanced.

We can think of the flatter islands in our model (11° facet angle) as the famous “hut” clusters discovered by Mo et al.,[41] and of the clusters with 60° facet angles as the “dome” clusters. It is well known that clusters with steeper side walls relieve the strain much more efficiently than the flatter clusters (see the discussion in Ref. [42]; the planar film, which is the limiting case of the flatter islands with a facet angle equal to zero, does not relieve the strain at all.) We see that large-angle facet islands affect more strongly the growth of the neighboring islands, leading thus to a more narrow size distribution.

We further conclude that a self-assembled population of quantum dots is expected at comparatively low temperatures such that the critical wetting-layer thickness for 3D islanding to take place approaches an integer number of monolayers. In InAs/GaAs quantum dots, the reported values of the critical thickness were found to vary from 1.2 to 2 monolayers,[43] (see also the discussion in Ref. [44] and the references therein). The critical wetting-
layer thickness should be given by an integer number of monolayers plus the product of the 2D island density and the critical volume (or area) $N_{12}$. The 2D island density increases steeply with decreasing temperature.[13] In such a case, a dense population of 2D islands will overcome simultaneously the critical size $N_{12}$ to produce 3D bilayer islands. The latter will interact maximally with each other from the very beginning of the 2D-3D transformation giving rise to a maximum wetting parameter and, in turn, to large-angle facets and a narrow size distribution. This is in agreement with the observations of Le Tanh et al. in the case of nucleation and growth of self-assembled Ge quantum dots on Si(001).[45] At 700°C, a population of islands with a concentration of the order of $1 \times 10^7 - 1 \times 10^8$ cm$^{-2}$ is obtained; the islands have the shape of a truncated square pyramid with four side wall facets formed by (105) planes with an inclination angle of about 11° and the size distribution of the islands is quite broad. On the other hand, at 550°C, a population of islands with an areal density of the order of $1 \times 10^9 - 1 \times 10^{10}$ cm$^{-2}$ is observed, the islands have larger angle (113) facets and their size distribution is much more narrow.

In summary, we have shown that the presence of neighboring islands decreases the wetting of the substrate (in this case the wetting layer) by the 3D islands. The larger the density of the array, the weaker the wetting. Neighboring islands with steeper side walls reduce more strongly the wetting of the considered island. The wetting parameter displays a maximum (implying a minimal wetting) when the array shows a monodisperse size distribution. We should expect optimum self-assembled islanding at lower temperatures such that the 2D-3D transformation takes place at the maximum possible island density.

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