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A model of strained epitaxy on an alloyed substrate

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Abstract

We propose a simple model of strained epitaxy with identical atoms being deposited on a substrate which is a disordered alloy. The model is aimed to be suitable for studies of experimentally observed complicated kinetics in such systems with the use of the Monte Carlo technique. Therefore, major attention is paid to the computational efficiency of the model. The techniques developed can be applied to one-dimensional (1D) as well as to two-dimensional heteroepitaxial systems with rectangular lattices of deposition sites. But for simplicity the formalism is presented mainly for 1D systems. In this case the model can be exactly solved at equilibrium with the use of the technique borrowed from the theory of protein folding. This is because in 1D the model of strained heteroepitaxy is equivalent to the Muñoz–Eaton model of protein folding. It is argued that at low temperature the model exhibits slow kinetics characteristic of glassy systems. The existence of the exact solution can be helpful in studying the approach to equilibrium in this complex system.

1. Introduction

The self-assembly of coherent nanostructures observed in some systems during strained epitaxy [1] is a subject of extensive current research. One of the major goals of this research is to develop techniques of controlled growth which is important in view of the potentially rich technological applications of coherent nanostructures [2]. One of the processes widely used to control the growth is the alloying both in the substrate [3, 4] and in the overlayer [5]. By changing the composition one usually aims to influence the misfit strain which is a major factor in the nanostructure self-assembly [6]. As a by-product, the attachment to the substrate and the kinetics are also strongly affected, which leads to complicated morphologies and kinetics of formation of heteroepitaxial overlayers [7]. The complexity of the processes observed experimentally is such that a rigorous interpretation is hardly possible without clear understanding of many competing processes underlying their behaviour.

The aim of the present paper is to propose a simple model of strained epitaxy on an alloyed substrate. Our major goal is to make the model appropriate for large scale Monte Carlo

simulations, so the approximations will be made to ensure computational efficiency. We achieve this by considering a rectangular geometry and the harmonic Frenkel–Kontorova model (FKM) used previously for studying the deposition on a pure substrate [8]. Because the two-dimensional (2D) generalization of our formalism in the case of the rectangular geometry is rather trivial [8], below we consider only the one-dimensional (1D) case which, besides being simpler for presentation, is also of practical interest in the studies of 1D heteroepitaxial phenomena [9–11]. The 1D model we consider is exactly solvable at equilibrium [12, 13] so the results of the MC simulations can be compared with the exact solution to check the approach to equilibrium. As we will see, this is a nontrivial question in the case of the deposition on a disordered substrate because in this case one may expect a considerable slowing down of the kinetics similar to that observed in glassy systems [14, 15]. This glassy behaviour introduces a new timescale which may seriously influence kinetic paths of self-organization phenomena.

2. The model

As we noted in the introduction, the lattice size misfit between the substrate and the growing overlayer is a major factor influencing both the overlayer growth mode and its morphology [6]. A simple approach to theoretical description of the misfit is provided by the 1D FKM which has frequently been used in qualitative [16, 17] and semi-quantitative studies [18, 19] of strained epitaxy. In the present paper we consider a modified FKM appropriate to coherent strained epitaxy on an alloyed substrate.

We consider an ensemble of a fixed number (N) of atoms coherently deposited on a 1D ‘surface’ which is a binary alloy consisting of two atomic species A and B. Let us first consider a model with the potential interactions between the atoms:

$$U = \sum_i n_i V_i(R_i + u_i) + \frac{1}{2} \sum_{ij} n_i n_j V(u_i + R_i - u_j - R_j),$$

where $R_i = ai$ (a the lattice constant, i any integer), $n_i = 0, 1$ is the occupation number of site i by an adatom, u_i the adatom displacement from the symmetric position R_i , V_i is the potential of interaction with the substrate near the site i , and V the interatomic potential. For simplicity we assume that the substrate potential $V_i(r)$ can take two values $V_A(r)$ and $V_B(r)$ as in a binary alloy. In reality the potential of an alloyed substrate is more complicated. For example, in the case of the deposition on the steps of the vicinal surfaces considered in [20] and [8] the deposited atom has five nearest neighbours, so even in the case of a disordered binary alloy the substrate potential will be a random mixture of five potentials. This, however, is a trivial complication which can be easily accounted for by considering a more complicated probability distribution of the substrate potential.

The analysis of the system considerably simplifies at low temperatures where it can be approximately reduced to a lattice gas model [8]. This is achieved by exploiting the fact that the residence time of atoms at the lattice sites can be arbitrarily large due to the Arrhenius law obeyed by the probability of activated hopping over the potential barriers separating neighbouring sites [21]. The dynamics of the variables u_i , on the other hand, do not have any energy barriers. So at sufficiently low temperature these variables are capable of reaching their thermal equilibrium distribution during the time intervals between the atomic hops, i.e., with the atomic configuration remaining unchanged. Averaging over u_i will leave us with an effective nonequilibrium free energy function F_{eff} of variables n_i only:

$$\exp(-F_{\text{eff}}/k_B T) = \int \prod_{\{n_i=1\}} du_i \exp(-U/k_B T). \quad (1)$$

This purely lattice model can be further used in both equilibrium and kinetic studies.

For the purposes of qualitative analysis it will suffice to average out the displacement variables in equation (1) in the harmonic approximation, i.e., by expanding V_i and V in the above equation up to the second order in the displacement variables u_i [18, 22] which is valid for small $|u_i|/a$. This reduces the integration in (1) to a multiple Gaussian integration which can be performed analytically (see below).

To facilitate comparison with other studies based on the FKM [16, 23, 17, 18] we write the harmonic approximation as the second order power series expansion in u_i for V_i and in $u_i - u_{i+1}$ for the pair potential V_p :

$$\begin{aligned} U &\approx \sum_i V_i n_i + \frac{1}{2} \sum_i n_i k_i u_i^2 + \frac{1}{2} \sum_{ij} n_i n_j V_{ij} + \frac{K}{2} \sum_i [(u_i - u_{i+1} - f)^2 - f^2] n_i n_{i+1} \\ &= \sum_i V_i n_i + \frac{1}{2} \sum_{ij} V_{ij} n_i n_j + \frac{K}{2} \sum_{ij} D_{ij} u_i u_j + Kf \sum_i u_i \nabla n_i n_{i+1} \end{aligned} \quad (2)$$

where V_i and V_{ij} are the values of the substrate and the pair potentials at the lattice sites for the atom in the symmetric position (the zero-order approximation); $f = -V'(a)/V''(a)$ (where V is the pair potential) is interpreted as the misfit parameter, the spring stiffness parameters $k_i = k_A, k_B$ and K are the second derivatives of the corresponding potentials, D_{ij} is the dimensionless dynamical matrix defined by this equality, and the discrete gradient ∇ is defined as $\nabla \phi_i \equiv \phi_i - \phi_{i-1}$. The most important simplification made in the above expansion is the assumption that the misfit parameter f is the same for all adatoms irrespective of the substrate atoms on which they reside. This approximation is crucial for our model because it allows us to reduce the calculation of the Green functions below to simple recurrence schemes (see the appendix). In the terminology used in the theory of disordered systems this approximation is usually called the approximation of diagonal disorder.

With approximation (2) the statistical average (1) amounts to Gaussian integration to give

$$\begin{aligned} F_{\text{eff}} &= \sum_i V_i n_i + \frac{1}{2} \sum_{ij} n_i n_j V_{ij} - \frac{k_B T}{2} \sum \ln \det(k_B T G) \\ &\quad - \frac{Kf^2}{2} \sum_i G_{ij} \nabla_i n_i n_{i+1} \nabla_j n_j n_{j+1}, \end{aligned} \quad (3)$$

where matrix G is the inverse of D . Assuming the system is aligned along the x -axis we ought to have also included the results of integration over the directions y and z . We do not discuss these contributions here because in the harmonic approximation they do not depend on the position of the atom in the system, so they are irrelevant to our present study. In cases of necessity these terms can be easily recovered. We also note the entropic contribution (the second term in the first line) which naturally appears in our formalism and which was shown to be crucial for proper description of the processes of deposition [24] as well as for the correct prediction of the shape of the atomic clusters [25].

Because of the gradient factors, only the ends of the contiguous chains of atoms contribute to the last term of equation (3), leaving three matrix elements of G_{ij} in the sum over ij inside every chain: two diagonal terms which we denote as $G_{11}^{(l)}$ and $G_{ll}^{(l)}$ (l being the chain length) and the matrix element $G_{1l}^{(l)}$ connecting the two ends of the chain. Furthermore, in the NN approximation the matrix D is block diagonal because the atoms belonging to different chains do not couple. Therefore, the determinant factorizes and the relaxation part of the free energy which consists of the terms in equation (3) containing G takes the form

$$F_{\text{relax}} = - \sum_{\text{chains}} \left\{ \frac{k_B T}{2} \ln \det[k_B T G^{(l)}] + \frac{Kf^2}{2} [G_{11}^{(l)} + G_{ll}^{(l)} - 2G_{1l}^{(l)}] \right\} \equiv \sum_{\text{chains}} E_l^{(i)}, \quad (4)$$

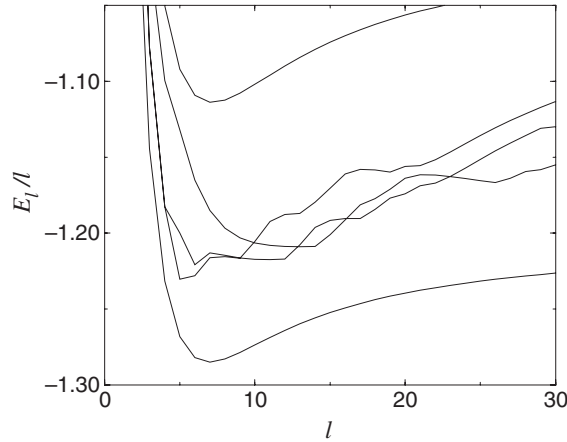


Figure 1. The chain energy per atom for pure substrates (the uppermost and the lowermost curves) and for three randomly generated configurations for equiatomic substrate composition.

where the summation is over the atomic chains by which we understand any contiguous atomic sequence surrounded by empty sites, including one isolated atom. The superscript (i) on E_l stresses that the system is not translationally invariant so all quantities pertinent to the chains depend on its exact placement. The same is true for the Green function elements $G_{ij}^{(l)}$ in which we omitted the above superscript to simplify notation.

3. Size calibration and kinetics

For concreteness, let us consider a system with the parameters similar to those found in the stressed Pt/Co system considered in [8]. Taking V_{NN} as the energy unit, the model will exhibit the size calibration if the Kf^2 is also equal to unity and $\alpha = 0.15\text{--}0.2$ with the calibrated chain length being equal to seven (see the uppermost and the lowermost curves in figure 1). Let us choose the substrate parameters as follows: $\alpha_A = 0.15$, $\alpha_B = 0.2$, $V_A = 0$ (the reference zero energy) and $V_B = -0.2$. The absolute values of V_i (with respect to the zero reference energy at the infinite separation) should be of the same order of magnitude as $V_{\text{NN}} = 1$ and their difference is assumed to be small because the substrate alloy is assumed to be random, so the atomic components should not differ too much in their physical properties. For the same reason the values of α_i are also chosen to be of similar magnitude. The value of α_A is lower than that of α_B because the harmonic part of the potential should be roughly proportional to its $r = 0$ value [17].

In deposition on a pure substrate the system exhibits self-assembly into size calibrated atomic chains provided the function E_l/l has a minimum at some finite value of l [26]. This can take place in the case when the misfit strain is sufficiently large [8]. In the case of an alloyed substrate it is reasonable to assume that locally the atomic chains will also try to minimize the $E_l^{(i)}/l$ ratio. But in this case the local atomic configuration of the substrate will not, as a rule, be the most favourable for the global energy minimization. In figure 1 we generated three random configurations corresponding to equiatomic substrate composition. It is seen that the chains self-assembled at a randomly chosen place on the substrate are very far from the absolute minimum of $E_l^{(i)}/l$ which corresponds to the value of the lowermost curve at $l = 7$. Therefore, at low coverage the chains will strive to reach this absolute minimum by seeking the places on the substrate where the B atoms are gathered together in rows of length greater than

or equal to seven. To reach this configuration the atomic chain in an unfavourable place should first disassemble into individual atoms and then seven of them should gather in the new ‘ideal’ place. We note that besides the energetic barrier at the first stage of decomposition, there also exists an entropic barrier because not only should the atoms assemble together in the new place but they also should arrive there in a sufficient quantity. This is because the optimum energy is the property of the whole ensemble of the chain atoms, not of an individual atom. Therefore, an atom may find a better place in a nonoptimum chain of the locally optimum length instead of a place in a chain which is fully placed on the energetically favoured B atoms but is not of the optimum length (which is seven in our case). We would like to stress that this behaviour is specific to the strained coherent epitaxy with the parameters satisfying the size calibration condition. In the case of incoherent structure, in view of the long time needed for the atomic chains to be assembled in the optimal places, the creation of dislocations would have been an easier way to release the strain energy.

In the case of high coverage there is no possibility for all deposited atoms to gather into the places on the substrate with 100% B-atom content. In the case of equiatomic substrate composition the probability of meeting at least seven B atoms in a row is of the order of $1/2^7$, so at the coverages exceeding $7/2^7 \approx 5.5\%$ the attachment places with nonoptimal compositions will also correspond to the global energy minimum. This poses a nontrivial problem of optimization which can hardly be solved by a simple enumeration in view of the large number of possible combinations.

According to the above picture equilibration kinetics of the system at low temperatures can proceed as follows. After a random deposition on the substrate the adatoms will gather in the clusters minimizing their $E_l^{(i)}/l$ ratio in the vicinity of a local energy minimum. Further evolution towards the global (free) energy minimum will proceed through the transitions of the chains over the local energetic barriers towards lower local energy minima. This picture is similar to that described in [15] where it was shown that this kind of energy landscape is common in many systems, such as glasses and proteins.

The analogy with the problem of protein folding is stressed by the fact that in 1D our model is formally equivalent to the Muñoz–Eaton [27] model of protein folding. This can be shown by mapping the relaxation energy (4) onto the lattice gas model as was done in [8, 13]. Namely, it is easy to show that F_{relax} can be expanded into an infinite sum of multiatom interactions [8]

$$F_{\text{relax}} = \sum_{i,l} V_l^{(i)} n_i n_{i+1} \cdots n_{i+l-1}, \quad (5)$$

where the upper index of $V_l^{(i)}$ indicates that the expansion coefficients which are given by the expression

$$V_l^{(i)} = E_l^{(i)} - 2E_{l-1}^{(i)} + E_{l-2}^{(i)} \quad (6)$$

are valid for all $l \geq 2$ with $E_0^{(i)} = E_1^{(i)} = 0$. In contrast to the translationally invariant case considered in [8, 13], in the present case the model with the Muñoz–Eaton type Hamiltonian

$$F_{\text{eff}} = \sum_i V_i n_i + \frac{1}{2} \sum_{ij} V_{ij} n_i n_j + F_{\text{relax}} \quad (7)$$

cannot be solved in the thermodynamic limit with the techniques developed in [13], and the method of paper [12] for finite systems should be used. Thanks to the constant- f approximation used by us the number of Green function matrix elements needed to compute all $V_l^{(i)}$ in the above equations is relatively low and can be generated using the recursive procedure described in the appendix for large size systems. The equilibrium quantities obtained with the use of the exact solution can then be compared to the results of the MC simulation to study the approach to the equilibrium which in glassy systems can be extremely slow [14].

4. Conclusion

In this paper we have developed a simple model of strained epitaxy which is capable of accounting for self-assembly of size calibrated clusters on alloyed substrates. We considered explicitly only the 1D case but the formalism developed can be straightforwardly generalized to 2D systems with a rectangular geometry of deposition sites. This is because the relaxations in the orthogonal directions are mutually independent and the formulae derived for one dimension can be applied to the two orthogonal directions without any modification [16]. In the case when there is anisotropy between the two directions only the parameters K and f should be appropriately adjusted.

Another modification of the model can be achieved in the MC simulations by introducing atomic kinetics into the substrate. The mobility of the surface atoms is usually much larger than the atomic diffusion in the substrate, therefore two competing timescales will appear: one for the slow glassy kinetics of the surface atoms in search of the most favourable configuration of the substrate atoms and another timescale due to the diffusion of the substrate atoms which can provide a local atomic rearrangement to minimize the energy. Depending on the relative efficiency of these competing processes one can observe different kinetics as well as changes in the local composition of the substrate and the morphology of the overlayer [4]. Further generalizations, such as accounting for the adlayer/substrate intermixing [28], are also possible in principle but they would spoil the computation efficiency of the model. Still, in the cases of intermixing of similar atoms, as in the Ge/Si case [28], one may expect some simplifications because, as our computations show, the Green function matrix elements are not very sensitive to small difference in the spring stiffness parameters.

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Appendix

According to equation (2)

$$D^{(l)} = \begin{pmatrix} 1 + \alpha_1 & -1 & 0 & \cdots & 0 & 0 & 0 \\ -1 & 2 + \alpha_2 & -1 & 0 & \cdots & 0 & 0 \\ 0 & -1 & 2 + \alpha_3 & -1 & 0 & \cdots & 0 \\ \vdots & \vdots & \ddots & \ddots & \ddots & \vdots & \vdots \\ 0 & \cdots & 0 & -1 & 2 + \alpha_{l-2} & -1 & 0 \\ 0 & 0 & \cdots & 0 & -1 & 2 + \alpha_{l-1} & -1 \\ 0 & 0 & 0 & \cdots & 0 & -1 & 1 + \alpha_l \end{pmatrix}, \quad (\text{A.1})$$

where $\alpha_i = k_i/K$. Because matrices $D^{(l)}$ are tri-diagonal, their determinants satisfy recurrence relations which can be used to calculate all quantities entering equations (4) and (6). The diagonal elements of the matrix $G^{(l)} = 1/D^{(l)}$ are

$$G_{ll}^{(l)} = r_{l-1} / \det D^{(l)}, \quad (\text{A.2})$$

where r_{l-1} is the determinant of the matrix obtained from $D^{(l)}$ by crossing out its last row and the last column:

$$r_{l-1} = \begin{vmatrix} 1 + \alpha_1 & -1 & 0 & \cdots & 0 & 0 \\ -1 & 2 + \alpha_2 & -1 & 0 & \cdots & 0 \\ 0 & -1 & 2 + \alpha_3 & -1 & 0 & 0 \\ \vdots & \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & \cdots & 0 & -1 & 2 + \alpha_{l-2} & -1 \\ 0 & 0 & \cdots & 0 & -1 & 2 + \alpha_{l-1} \end{vmatrix}. \quad (\text{A.3})$$

Expanding $\det D^{(l)}$ with respect to the last row we get

$$\det D^{(l)} = (1 + \alpha_l)r_{l-1} - r_{l-2}. \quad (\text{A.4})$$

Comparing this with equation (A.2) we get

$$G_{ll}^{(l)} = 1/(1 + \alpha_l - d_{l-1}), \quad (\text{A.5})$$

where $d_{l-1} = r_{l-2}/r_{l-1}$. Now, expanding the determinant (A.3) with respect to the elements of the last row we get the following three-term recurrence relation:

$$r_{l-1} = (2 + \alpha_{l-1})r_{l-2} - r_{l-3}. \quad (\text{A.6})$$

But because equation (A.2) includes only the ratio r_{l-2}/r_{l-1} , by dividing equation (A.6) by r_{l-2} we can transform it to a simpler form

$$\frac{1}{d_{l-1}} = 2 + \alpha_{l-1} - d_{l-2}. \quad (\text{A.7})$$

The off-diagonal matrix element $G_{ll}^{(l)}$ of the inverse matrix $G^{(l)}$ is equal to the ratio of the determinant of the matrix obtained from $D^{(l)}$ by crossing out its last row and the first column multiplied by $(-1)^{l+1}$ and divided by $\det D^{(l)}$. As is easy to see from equation (A.1), the matrix thus obtained is a triangular matrix with the diagonal elements all being equal to -1 . Hence its determinant is equal to $(-1)^{l-1}$ and

$$G_{ll}^{(l)} = 1/\det D^{(l)} = \det G^{(l)}. \quad (\text{A.8})$$

From equation (A.4) we get

$$G_{ll}^{(l)} = \frac{1}{\det D^{(l)}} = \frac{1}{r_{l-1}(1 + \alpha_2 - d_{l-1})} = \frac{b_{l-1}}{1 + \alpha_2 - d_{l-1}} = b_{l-1}G_{ll}^{(l)}, \quad (\text{A.9})$$

where $b_{l-1} = 1/r_{l-1} = d_{l-1}b_{l-2}$ (see the definition of d_{l-1} above). Finally, making the shift $l - 1 \rightarrow l + 1$ the above formulae can be summarized as

$$\begin{cases} G_{ll}^{(l+1)} = 1/(1 + \alpha_{l+1} - d_l) \\ G_{ll}^{(l+1)} = \det G^{(l+1)} = G_{1,l+1}^{(l+1)}b_l, \end{cases} \quad (\text{A.10})$$

where d_l and b_l are generated by the recursion relations

$$d_{l+1} = 1/(2 + \alpha_{l+1} - d_l) \quad \text{and} \quad b_{l+1} = d_{l+1}b_l \quad (\text{A.11})$$

initialized by $d_0 = b_0 = 1$. The matrix element $G_{11}^{(l+1)}$ is calculated in the same way by starting the recurrence from the upper left corner of the matrix $D^{(l+1)}$. The matrix element $G_{ll}^{(l+1)}$ is equal to $G_{ll}^{(l+1)}$ due to the symmetry.

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