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Step bunching and macrostep formation in 1D atomistic scale model of unstable vicinal crystal growth

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ABSTRACT

We devise a new 1D atomistic scale model of vicinal growth based on Cellular Automaton. In it the step motion is realized by executing the automaton rule prescribing how adatoms incorporate into the vicinal crystal. Time increases after each rule execution and then n_{DS} diffusional updates of the adatoms are performed. The increase of n_{DS} switches between the diffusion-limited (DL, n_{DS}=1) and kinetics-limited (KL, $n_{DS} > > 1$) regimes of growth. We study the unstable step motion by employing two alternative sources of instability – biased diffusion and infinite inverse Ehrlich-Schwoebel barrier (iiSE). The resulting step bunches consist of steps but also of macrosteps since there is no step-step repulsion incorporated explicitly into the model. This complex pattern formation is quantified by studying the time evolution of the bunch size N and macrostep size N_m in order to find the proper parameter combinations that rescale the time and thus to obtain the full time-scaling relations including the pre-factors. For the case of biased diffusion the time-scaling exponent β of N is 1/2 while for the case of iiSE it is 1/3. In both cases, the time-scaling exponent β_m of N_m is ~$3\beta/4$ in the DL regime and $3\beta/5$ in the KL one.

1. Introduction

The production of new devices nowadays reaches new frontiers of miniaturization but these fast and dramatic changes require very precise tuning of layer-by-layer (step-flow) crystal growth. Thus, the detailed use and directed manipulation of the processes and patterns on atomic scale is of crucial practical relevance. For this, it is necessary to reach a fundamental understanding of the growth mechanisms and their consequences on atomic scale. This is why the surface morphologies resulting from various kinds of crystal growth processes are subject of interest for large groups of researchers [1–5]. Surface self-organization resulting in well-ordered structures is used to build templates for growing nano-scale objects such as nano-dots or nano-wires [6,7]. It is known that at the miscut surfaces the asymmetry between adatom fluxes which attach to the steps from above and bottom terraces leads to surface instabilities [8–12]. If the amount of particles attaching to the step from the lower terrace is higher than the particle flux from the above terrace meandered patterns emerge [10]. Otherwise, when the flux incoming from above is higher a step bunching process happens [10,13]. Flux asymmetry at steps can be induced by various dynamic mechanisms. The most often discussed in this context are biased adatom diffusion i.e. due to electromigration [10,14] or the existence of an Ehrlich-Schwoebel barrier (SE) [1,3–5,15]. Below we will concentrate on these two sources of surface instability.

The mechanism of step bunching that happens due to each of these instability sources has been widely discussed and analyzed in its various aspects [1,3–5,13–18]. Its initial stages, starting from step doubling are easy to observe and analyze. However, when coming to an exact evaluation of the scaling factors it is necessary to ensure large systems, many samples and long times of study. This is very difficult in experimental systems [14] and in more realistic MC simulations as well [5,10]. Analytic models give better chance [10,17–22], however it would be good to link their parameters with the ones of discrete systems. From the other side classification of the studied phenomena to the proper universality class [19] is a good course to understand mechanisms and character of this dynamical process. In this work, a model based on cellular automata (CA) is studied as a simple, clear, and powerful tool that is expected to be able to go beyond the analytical treatments. By extensive investigations of the proposed model in one dimensional system we are able to determine different scalings of the bunch size N with time in the regime of intermediate asymptotics [23].

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In the case of biased diffusion we get scaling exponent β=1/2 and in the case of the surface with infinite inverse Ehrlich-Schwoebel barrier (iiSE) it is β=1/3. The step bunches we observe in our simulations consist of single steps that have size of one unit cell, but also of macrosteps with size of multiple unit cells. Such formations are seen in experiments [24] and their time evolution remains subject of studies [25,26]. Macrosteps are created during the surface evolution process because there is no step-step repulsion incorporated into the model. This complex pattern formation is analyzed and together with the scaling of bunch size N the time dependence of the size of macrosteps N_m is studied. In both variants of the model the time scaling exponent β_m of N_m is reduced o approximately $3\beta/4$ of the scaling exponent of N in the DL regime and $3\beta/5$ in the KL one. We find also the proper parameter combinations that rescale the time and as an effect, all studied curves are collected along a universal one.

Both studied systems allow to investigate scaling in wide range of parameters. Preliminary results presented in [27] have shown some examples of the scaling behavior. Now we expand our analysis into other areas of parameters and show how results for wide range of model parameters scale along universal curves. We checked that different bias values give the same scaling. More interestingly, in the system with iiSE the data for the bunch size also scales along the same line in both slow and fast diffusion limits.

Below the model is described, then we show and analyze time scaling for step bunch sizes and macrostep sizes for both studied systems. General scaling functions are shown and discussed. We also compare step profile forms as an effect of biased diffusion and the presence of iiSE at the step.

2. The model

The model is devised as the simplest possible proposition that is able to achieve atomic scale resolution while still retaining the possibility for fast calculations on large systems. It is built as a combination of two modules: the deterministic one – a cellular automaton (CA) and a diffusional module - a typical Monte Carlo (MC) procedure that brings the concept of stochasticity into the model still keeping track of the positions of the individual adatoms. Each cell from the 1D colony is given a value equal to its height in the vicinal stairway that descends from the left to the right. In the beginning, the steps are regularly distributed at distance l_0. Another 1D array of the same size L contains the adatoms. In the beginning they are randomly distributed over the surface with concentration c. The growth rule defines that each time there is an adatom at the right nearest neighboring site to a step or macrostep it attaches unconditionally to it. Then the step or the lowest layer of the macrostep advances one position to the right, which is realized by increasing the value of the vicinal cell colony at the position of the adatom by one as, illustrated in Fig. 1. The adatom is deleted from the adatom array. The growth updates using the growth rule are performed in a parallel fashion – the update (change of height at that position with 0 or 1) of each cell from the vicinal crystal is kept aside in a mirror array while every cell is checked, then the whole cell population is renewed at instance using this mirror array and only then the time is increased by 1. Each execution of the automaton rule is complemented by compensation of the adatom concentration to c and the adatom population is then subjected to diffusional update(s) in a serial manner, their number being denoted by n_{DS}. In any diffusional update a total number of adatom positions equal to the size of the adatom array L is chosen sequentially at random. Then, if an adatom is found there, it is tried to let it jump left or right with some probabilities, usually their sum being 1, except in the case of iiSE, and the move is accepted only if the next chosen adatom position is not occupied already by an adatom. The change of this adatom's position is enforced without postponing and another position is checked for availability of an adatom. These diffusional updates do not contribute to increase of the time. Thus, with increasing n_{DS} a transition is realized from diffusion-limited (DL) growth to a kinetics-limited (KL) one – while the kinetic events (growth rule executions) happen with the same fixed frequency and the diffusing adatoms can make on average as many hops as determined by n_{DS} before being eventually captured by the growing surface [28]. The diffusion is influenced by one of two principal sources of instability – directional bias or iiSE. The bias is realized by defining that the hop probability to the right is (0.5+δ) while to the left it is (0.5−δ). The iiSE is realized through inhibition of the diffusional hops to the left when the adatom is the right next nearest neighbor to a step or macrostep and inhibition of the diffusional hops to the right when the adatom is the left nearest neighbor to a step or macrostep. Thus the only source of adatoms incorporating into a step is the terrace behind it plus a small amount that remains to the left of the infinite ES barrier when re-building it one lattice site to the right in the process of discrete step motion. The growth rule for iiSE case is presented in Fig. 1b. Adatom diffusion over the barrier outlined there is blocked. Note the iiSE turns the model into one-sided. Destabilizing factors in the model are not opposed by step-step repulsions, hence there is no factor preventing the formation of macrosteps. Indeed as it will be shown later step bunches in fact are built out of macrosteps that become dominating structure visible in the profile of the crystal.

The model permits fast calculations on systems with large sizes thus achieving the regime of intermediate asymptotics [23] where a reliable statistics is collected for the monitored properties. In order to control the developing surface patterns we adopt a modification [27] of an established monitoring protocol [29]. It is the formation of macrosteps that determines the need of this modification. We investigate the time dependent bunch size N and macrostep size N_m, which are the parameters useful for the description of the step bunching phenomenon. An important criterion built into the protocol defines when two neighboring steps belong to the same bunch – it is when the distance between them is less than l_0, whereas groups of steps with distance l=0 are considered as macrosteps. The bunch size N measures the height interval between the topmost bunch step and the lowest one. The same approach is applied to the macrostep size N_m. In the numerical results presented below bunch usually consists of steps and macrosteps as well (see Fig. 2). To obtain proper scaling of the results presented below we performed calculations for large systems (up to 180,000 sites), large number of time steps (~10^8) and usually repeat calculations at least 5 times each.

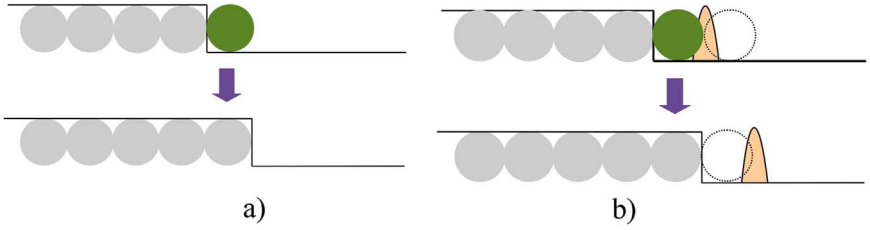

Fig. 1. Step move as an effect of CA module incorporation of diffusing particle into the step (a) in the biased diffusion model and (b) in the system with iiSE. It can be seen how the infinite ES barrier is removed from the place where it is established and re-established at one lattice position to the right.