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Inverted List Kinetic Monte Carlo with Rejection Applied to Directed Self-Assembly of Epitaxial Growth

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Abstract. We study the growth of epitaxial thin films on pre-patterned substrates that influence the surface diffusion of subsequently deposited material using a kinetic Monte Carlo algorithm that combines the use of inverted lists with rejection. The resulting algorithm is well adapted to systems with spatially heterogeneous hopping rates. To evaluate the algorithm's performance we compare it with an efficient, binary-tree based algorithm. A key finding is that the relative performance of the inverted list algorithm improves with increasing system size.

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1 Introduction

A typical Kinetic Monte Carlo (KMC) [1, 3, 5, 7] model/simulation of epitaxial growth features a small set of distinct rates related to a corresponding small set of different local environments. KMC simulations become more complex, however, when the number of distinct rates becomes large. Such situations arise, for example, when there is strain in the system, or more generally, when the potential energy surface (PES) is varying continuously.

In this paper, we implement an efficient KMC algorithm [13] that effectively handles arbitrary rate distributions through a combination of rejection and inverted list techniques. This generalizes the well-known Bortz-Kalos-Lebowitz (BKL) [3] algorithm. A

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key feature of the BKL "N-Fold way" is the use of a binning strategy along with what we refer to as "inverted lists". Briefly, if a list $\{e_k\}$ stores the spatial location of an event at (i,j) in memory location k, an inverted list $\{e_{(i,j)}\}$ allows one to quickly perform the reverse operation of identifying the memory location corresponding to the event at (i,j). This type of data structure is needed to efficiently rearrange the events within the bins after an event is executed. This feature is easily overlooked in the original work, however, and, without the inverted lists, a binary tree algorithm [2] is faster—scaling like $\mathcal{O}(\log N)$, where N is the number of independent random events to be sampled from. In an earlier publication, Schulze [12] points out that an inverted-list BKL algorithm has an operation count that is fixed as the system size N increases and compares the practical performance of the two algorithms in the frequently occurring special case where there is a small number, $M \ll N$, of distinct rates.

When combined with rejection, the inverted list technique requires one to partition the rates into M categories, the boundaries of which must be chosen by the user so as to keep the rejection percentage low. There is a tradeoff between the reduced rejection offered by increasing the number of categories and the increased cost of searching through additional categories. This is the first work to fully implement and study the performance of the combined algorithm and we have two aims:

1. give an example of a physical system where such a generalization is needed.
2. demonstrate that the partitions can be chosen so that the inverted list algorithm outperforms the binary search.

As an example of a situation calling for the generalized algorithm, we take up the study of directed self-assembly during epitaxial growth, as recently modeled by Niu et al. [9], who used an island dynamics model and the level-set technique. This continuum approach is based on the seminal work of Burton-Cabrera-Frank (BCF) [4]. The authors show that regular arrays of nano patterns can be obtained if the PES for surface diffusion is varied. Such variations can, for example, result from buried defects [6], and the subsequent long-range strain field in the substrate. We also offer a few comments on the tradeoffs between the continuum and atomistic models. As a rule, atomistic simulations allow for a more faithful description of all relevant microscopic processes, but, as a result, are limited to smaller length and time scales.

In the first section of this paper we briefly review the model and the KMC algorithm. In the second section we compare results obtained from the KMC simulations with the recent results of Niu et al. [9] and illustrate some additional situations that can be addressed using KMC. In the final section we compare the performance of the inverted list with rejection KMC algorithm with a binary-tree based algorithm [2].

2 Growth model and KMC algorithm

Before presenting the results of our simulations, we briefly discuss the KMC algorithm. KMC simulation of surface evolution requires one to keep track of possible events which