Parallel molecular dynamics simulations of deposition processes

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Abstract

The design of production processes for new materials with improved physical properties requires a subtle modeling, simulation, and model verification by experimental data. Here, we consider specific deposition processes for the production of innovative materials such as boron nitride and silicone carbide to be used in semiconductor technology. Emphasis is on Molecular Dynamics (MD) simulations and implementation of the mD algorithms on parallel platforms as the IBM SP2 of the LRZ, Munich.

Keywords: Molecular dynamics; deposition processes; parallel algorithms

1 Introduction

In semiconductor technology, in particular for high power and high temperature devices, new materials such as cubic boron nitride (c-BN) and silicon carbide (SiC) are of utmost importance due to their improved physical properties (large bandwidth, high saturation drift velocity, excellent thermal conductivity). The layout and design of innovative production processes involving e.g. codeposition of fullerenes (C_{60}) on Si substrates (cf. [3, 4]) resp. ion beam assisted deposition of boron nitride (cf. [2, 4]) require a proper mathematical modeling of the dynamics of the surface growth processes and an adequate simulation by efficient numerical techniques. Molecular Dynamics (MD) modeling and simulation (cf. [1] - [4]) are appropriate tools to study the interaction of the depositing particles with the substrate resp. the already formed surface layer. Due to the large number of particles that have to be taken into account for realistic simulations, the development and implementation of parallel algorithms play significant roles in order to achieve reasonable computational times.

2 Numerical and Computational Aspects

The MD modeling involves Newton's equations of motions

$$\begin{aligned} m_i \, d\,\mathbf{v}_i/d\,dt &= -\nabla_{\mathbf{r}_i} V(\mathbf{r}_1, \cdot, \cdot, \cdot, \mathbf{r}_N) \\ d\,\mathbf{r}_i/d\,dt &= \mathbf{v}_i \quad , \quad 1 \le i \le N \end{aligned}$$

where the potential V describes the atomic interactions with respect to the entire range of possible configurations. For the deposition of c-BN and fullerene carbonization, suitable choices are the so-called Tersoff- resp.

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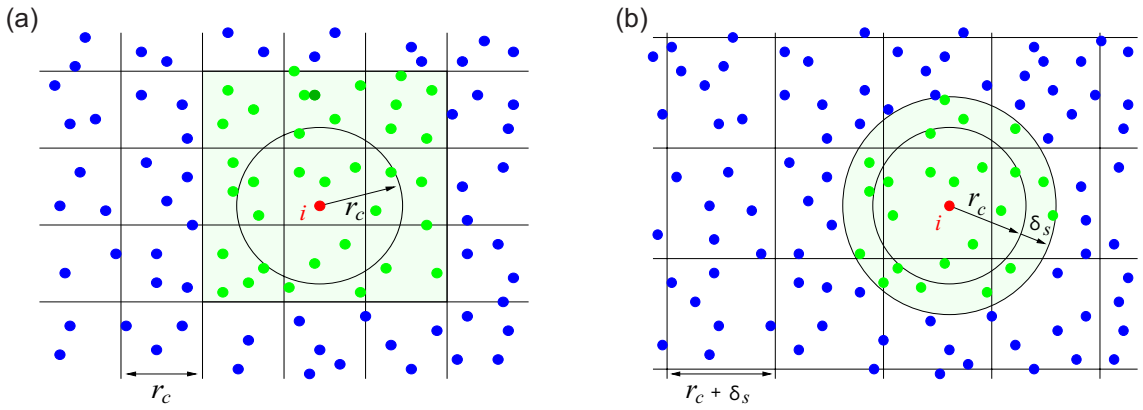

Figure 1: (a) Particle-In-Cell Method, (b) Verlet-Neighbor-List

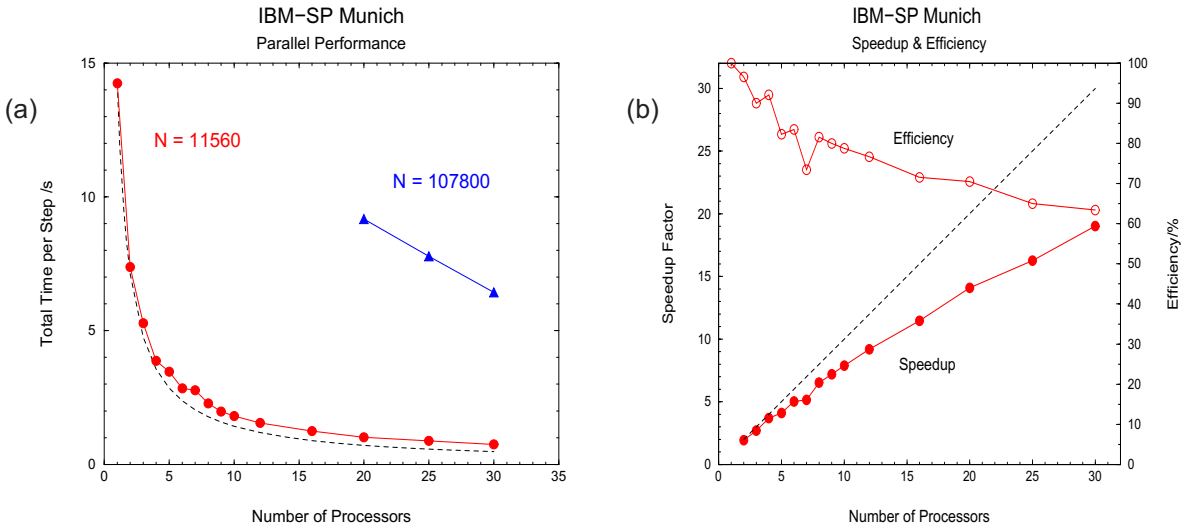

Figure 2: (a) Parallel Performance, (b) Speed-Up & Efficiency

Brenner-Tersoff potentials (cf. [2] - [4]).
In particular, the Tersoff potentials are of the form

$$V \;=\; \frac{1}{2}\sum_{i\neq j} V_{ij} \;=\; \frac{1}{2}\sum_{i\neq j} f_C(r_{ij})\,[\,f_R(r_{ij}) \;+\; b_{ij}\,F_A(r_{ij})\,]$$

with a cut-off function $f_C(\cdot)$ and attractive/repulsive potentials $f_A(\cdot)$ and $f_R(\cdot)$ (see [2] for details).
A bond-order-concept is used in the sende that the more neighbors an atom has, the weaker the bond to each neighbor is:

$$b_{ij} \;:=\; (\,1 \;+\; \beta^n\,\xi_{ij}^n\,)^{-1/2n} \quad , \quad \xi_{ij} \;:=\; \sum_{k\neq i,j} f_C(r_{ik}) \;\;.$$

Parameters are fitted on the basis of ab-initio quantum mechanical calculations.
The Verlet scheme has been used for numerical integration which is a symplectic method of order 2 (cf. [1]).

3 Parallelization and Performance

A parallel version of the Verlet method has been implemented on the IBM SP2 using a particle-in-cell approach and the nearest neighbor concept based on the distribution of the cells to the available processors. Figures 2a and 2b display the parallel performance (Fig. 2a) and the speed-up & efficiency (Fig. 2b) of the parallelized Verlet scheme.

4 Remarks and References

For further information see URL: http://wwwhoppe.math.uni-augsburg.de/index.html

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