Parallel Molecular Dynamics Simulation of Sputter-Deposition Thin-Film Growth

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The purpose of this work is to use parallel scheme to improve the computational efficiency of MD simulation [1] of thin-film morphology in the sputtering process [2], such that the number of atoms can be increased. Advanced technique is used to reduce the elapsed time for simulating the problem. The procedure of thin-film deposition process is divided into three procedures [3]. First, we initialize simulating atoms, includimg incident atoms, thermostated atoms and anchor atoms. The anchor atoms are to prevent the substrate from being distorted by incident atoms during deposition. The thermostated atoms are to hold the substrate at desired temperature. The above two kinds of atom are arranged by face-center-cubic (FCC) crystalline structure initially because copper atom is used in our program (see Fig. 1). In simulating process the incident atoms will be deposited on the substrate. The positions of the atoms are provided randomly on the x direction and the velocities are given by incident kinetic energy. Second the forces between atoms are calculated in equilibrating procedure. In this program the Verlet-Velocity scheme [4] is used to integrate the equation of the motion and the potential between atoms is of Lennard-Jones type. For saving simulating atoms we use periodic boundary condition. The temperature of the system changes when the incident atoms interact with the atoms of substrate, and is not suitable for physical condition. So one needs to rescale the temperature to desired temperature. The final procedure is thin-film production. We assume that the incident atoms don't interact each other before one of the atoms interacts with the atoms of substrate. The morphologies of films for different physical parameters, such as temperature, incident energy, and deposition rate are studied.

For parallel computing technique, we implement spatial domain-decomposition scheme [5]. The physical domain to be simulated is partitioned into some sub-domains of equal volume that the geometry of each sub-domain is uniform (structured computing grid). Assign sub-domains into a processor and the coordinate of processor is Cartesian topology [6]. The atoms will communicate between processors in simulating process. There are two steps for calculating forces; one is mapping the atoms, its position less than cutoff region, to the corresponding processors for calculating forces [7]. The other step is that after force calculation, the atoms have new coordinate and we need to assign the atoms to corresponding processor again.

For computing facility, we install PC Cluster parallel computing architecture, because it is cheaper and scalable. On each computational node one has Intel Pentium IV microprocessor with speed 1.7MHz and the memory is Rambus 400MHz of 512Mbytes and network interface card is fast Ethernet with bandwidth 100Mb/sec (see Fig. 3). The communicating protocol is based upon the Message Passing Interface (MPI) [8].

The result of deposition of 2D and 3D sputtering processes are shown in Fig. 3 and Fig 4. The elapsed time of 2D case is significantly reduced. In Fig 5a, the speedup curve is linearly proportional to the number of CPUs. According to our work the complexity of elapsed time will be reduced from $O(N^2)$ to $O(N^2/p)$, where p is the number of CPUs and N is number of simulating atoms.

In the full paper, more detailed information about the numerical scheme, parallel implementation and additional results will be included. First, we will implement different potential functions, Embedding-Atom method (EAM) [9], which allow one to manipulate multi-

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component alloy metal. In MOS fabrication, copper and titanium atoms are used for interconnecting process. The other result is to implement unstructured grid to achieve load-balance that is important for multi-scale simulation for nano- technology computing.

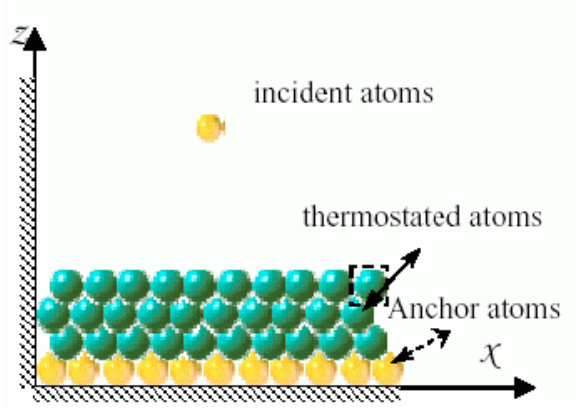

Fig. 1. Initial arrangement of atoms

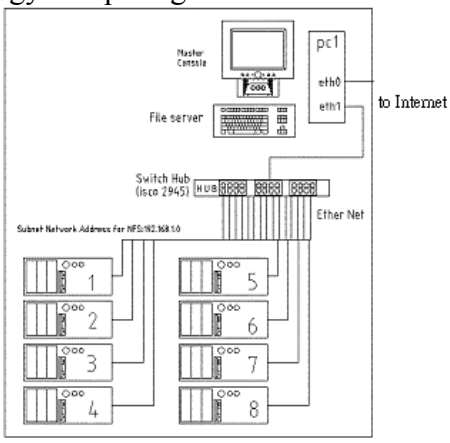

Fig. 2. Layout of computing facility

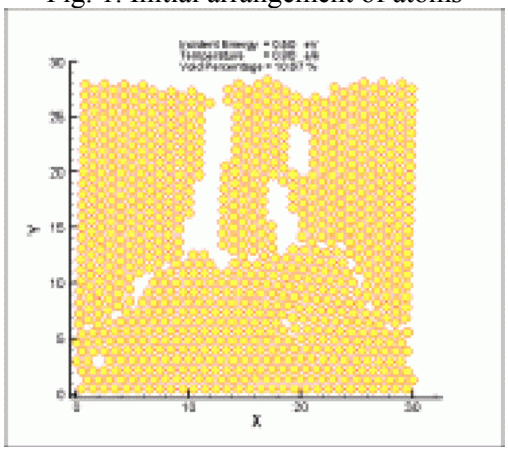

Fig. 3a. Thin-film deposition

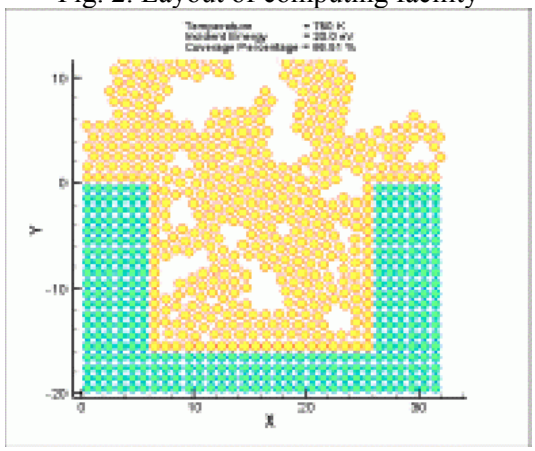

Fig. 3b. Trench-filling deposition

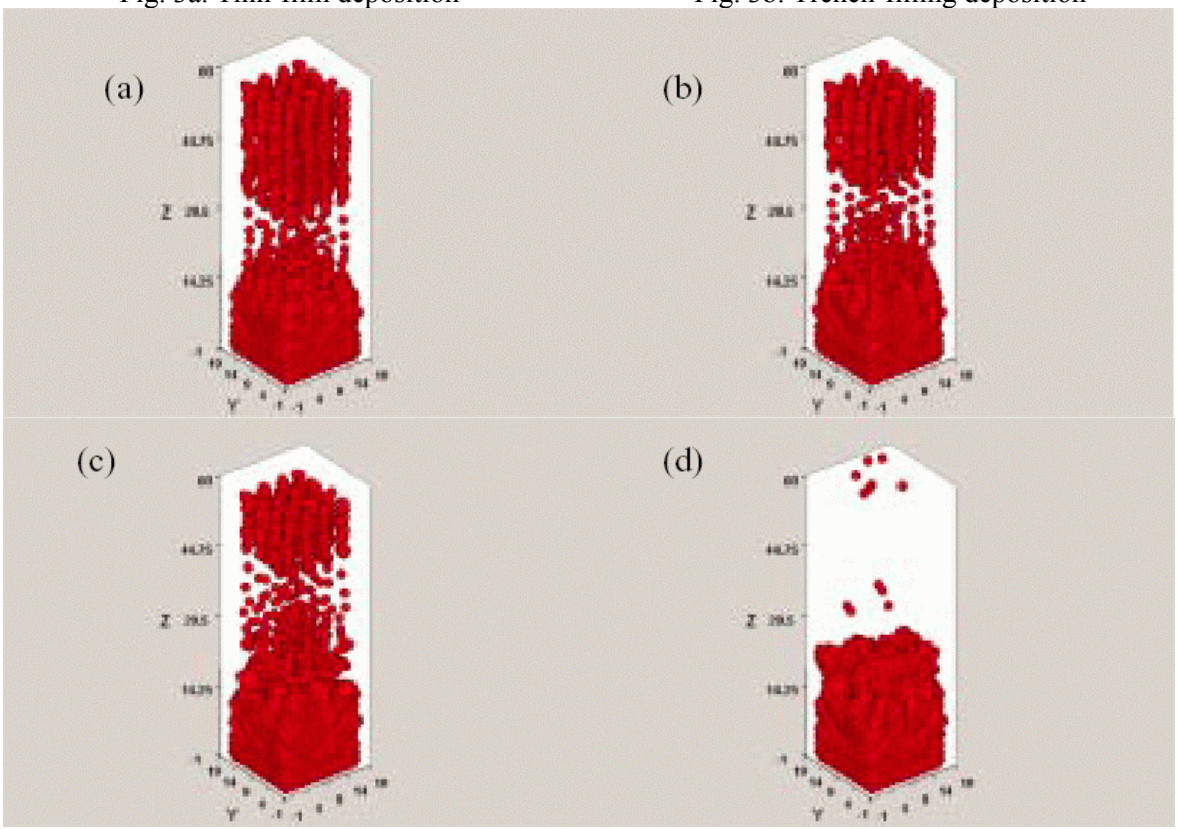

Fig. 4. The snapshot of deposition process(9600 atoms) (a). 40 time step. (b) 80 time step. (c) 120 time step. (d) 180 time step.

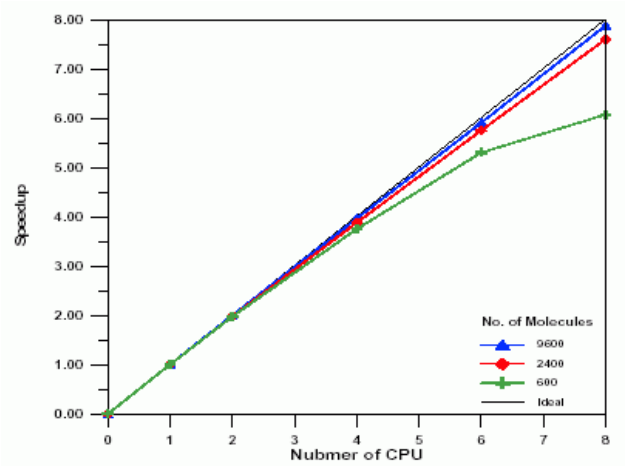

Fig. 5a. speedup .vs. number of CPUS

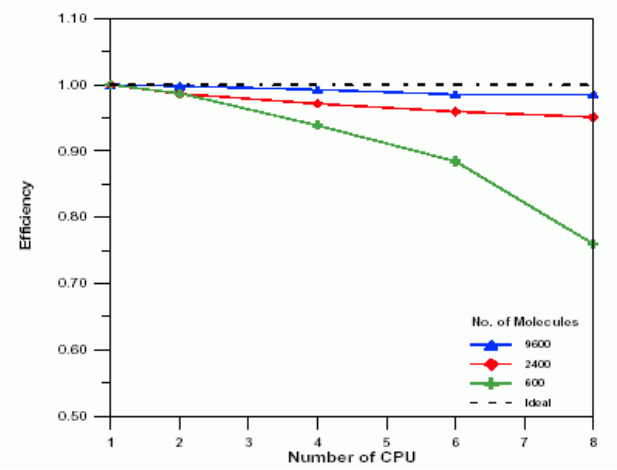

Fig. 5b. efficiency .vs. number of CPUs

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