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High-performance Full-atomistic Simulation of Optical Thin Films

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The experimental study of the dependence of thin film properties on the deposition conditions may be still a great challenge. Today the progress in high performance computing allows one to perform the investigation of these dependencies on the atomistic level using the classical molecular dynamics (MD) simulation. In the present work the computational cost and efficiency of classical full-atomistic simulation of thin film deposition process using the Lonmonosov-2 supercomputer facilities is discussed. It is demonstrated that using 512 computational cores of the Lomonosov-2 supercomputer ensures the simulation of thin film cluster with technologically meaningful thickness of an optical film. Because of a relatively slow growth of the simulation time with the increase of film thickness we guess that simulations clusters with thicknesses that are several times higher than the currently achieved thicknesses about one hundred nanometers is quite realistic if the number of available computational cores will be increased up to several thousands.

Keywords: thin film structure, deposition process, molecular dynamic simulation, silicon dioxide.

Introduction

Optical thin films and coatings are important components of almost all modern optical and optoelectronic instrumentation. The detailed knowledge of the dependence of thin film structural properties on parameters of film deposition process is a key to a further progress in thin film technology. Experimental study of thin film microscopic structure may be still a great challenge. At the same time the progress in high performance computing allows one to perform the investigation of thin films properties on the atomistic level using the classical molecular dynamics (MD) simulation [1]. The MD-based approach for the simulation of deposition of thin films clusters with thicknesses up to hundreds of nanometers was recently developed and was successfully applied to the detailed investigation of silicon dioxide films [2–5].

In the present paper the current status and further prospects of the high-performance investigation of structural and mechanical properties of optical thin films are briefly discussed.

1. Simulation Method

The simulation of the silicon dioxide thin film deposition is organized as a step-by-step procedure [2–5]. At every deposition step, SiO_2 groups are injected at the top of the simulation box and are directed to the film surface. Duration of every deposition step is enough to ensure the formation of chemical bonds between the film and injected atoms. All atoms inside the simulation box move in agreement with the Newton laws. Their interactions are described in the frame of the DESIL force filed [2] that was specially developed for the simulation of the deposition process. The research is carried out using the equipment of the shared research facilities of HPC computing resources at Lomonosov Moscow State University. Simulation of the deposition process is performed using parallel KUVALDA program [2], for MD part of the algorithm the GROMACS package [6] is used.

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2. Results and Discussion

The time of MD simulation of one injection cycle depends linearly on the number of deposited atoms N_{at} and the total time of the deposition process simulation is proportional to the square of the N_{at} [2]. This is a reason for a relatively high computational cost of the simulation procedure as compared to the MD simulation of clusters consisting of fixed numbers of atoms.

Dependencies of the simulation time on the number of the deposited atoms are shown in Fig. 1.

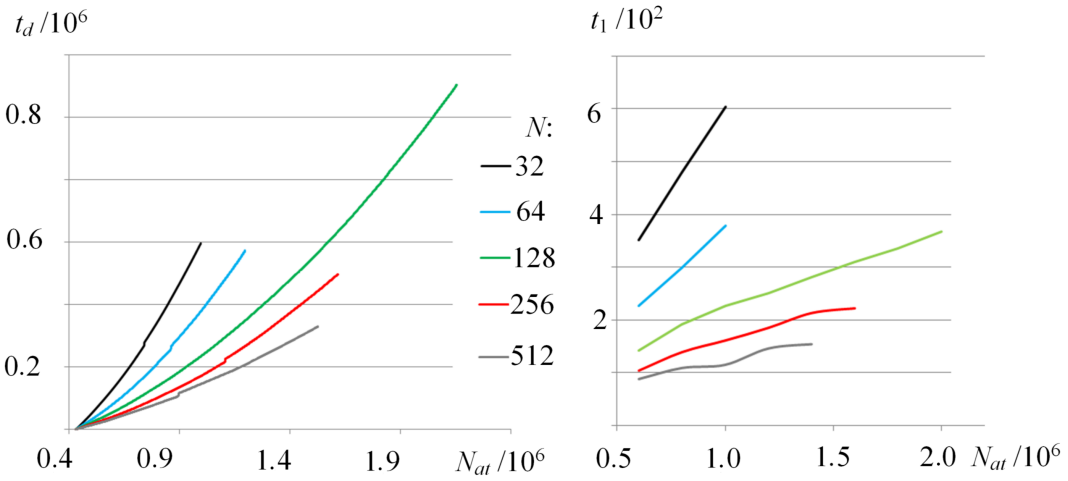

Figure 1. Dependencies of the full deposition time $t_d(s)$ and duration of one deposition cycle $t_1(s)$ on the number of deposited atoms N_{at} for different numbers N of computational cores

It is seen from Fig. 1 that using 512 computational cores of the Lomonosov-2 supercomputer ensures the simulation of thin film cluster with approximately 1.5×10^6 atoms which corresponds to the technologically meaningful thickness of an optical film. The simulation time in this case is about three days. But this makes possible a systematic investigation of thin film properties. It is interesting that the duration of one deposition cycle increases slowly with the growth of the number of deposited atoms (right part of Fig. 1). Because of a relatively slow growth of the simulation time with the increase of film thickness, we believe that simulations of film clusters with thicknesses that are several times higher than the currently achieved thicknesses is quite realistic if the number of available computational cores will be increased up to several thousands.

When the deposition process is over, film properties such as density profiles, point defects concentration, surface roughness, mechanical stress, Young modulus, etc. can be investigated [7]. Investigation of these properties requires MD simulations with the durations of hundreds of picoseconds. The results of the investigation of the computational cost of these simulations are shown in Fig. 2. Multi-core efficiency is calculated as:

$$a = (t_{32}/t_N)(N/32), \tag{1}$$

where t_{32} and t_N are the simulation times for the same cluster when 32 and N cores are used respectively. Although the efficiency is reduced with the growth of N (Fig. 2), the parallel computations with $N = 512$ and 1024 ensure a systematic study of film structural properties for the clusters with thicknesses of about 100 nm. It is clearly seen from the comparison of the results presented in Fig. 1 and Fig. 2 that the simulation of deposition process is the most time-consuming part of the investigation of thin film properties.

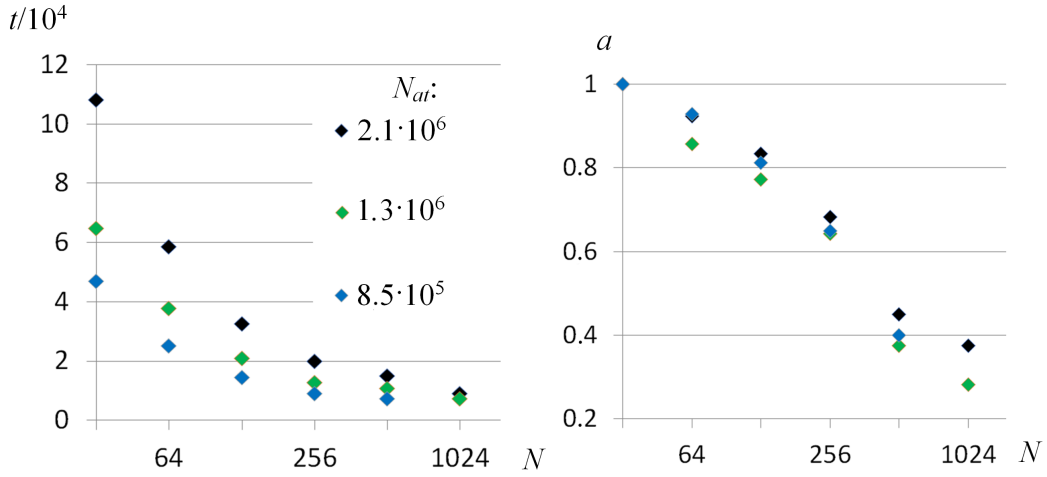

Figure 2. Dependencies of the simulation time $t(s)$ and multi-core efficiency a on the number of computational cores N; N_{at} is the number of atoms in the deposited cluster. Duration of the MD trajectory is 1 ns

Conclusions

Currently available computational resources of the Lomonosov-2 supercomputer are sufficient to the systematic full-atomistic investigation of structural and mechanical properties of optical films with technologically meaningful thicknesses of about a quarter of visible light wavelength. Simulation of the deposition process is the most time-consuming part of the investigation. Increasing the number of computational cores up to several thousand will make possible a full-atomistic simulation of coatings with several thin films.

Acknowledgments

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