High-performance Atomistic Simulation of the Annealing of Ta_2O_5 Thin Films

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ТОНКИЕ ПЛЕНКИ

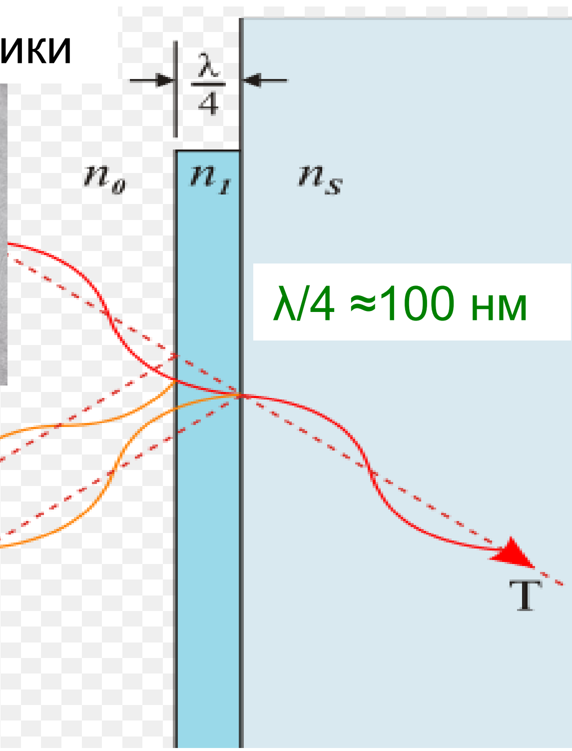
Применение:
Мобильные телефоны, видео-фотокамеры, архитектурное стекло, очки, фильтры, зеркала, линзы…

Изготовление:
напыление в вакуумной камере на подложку

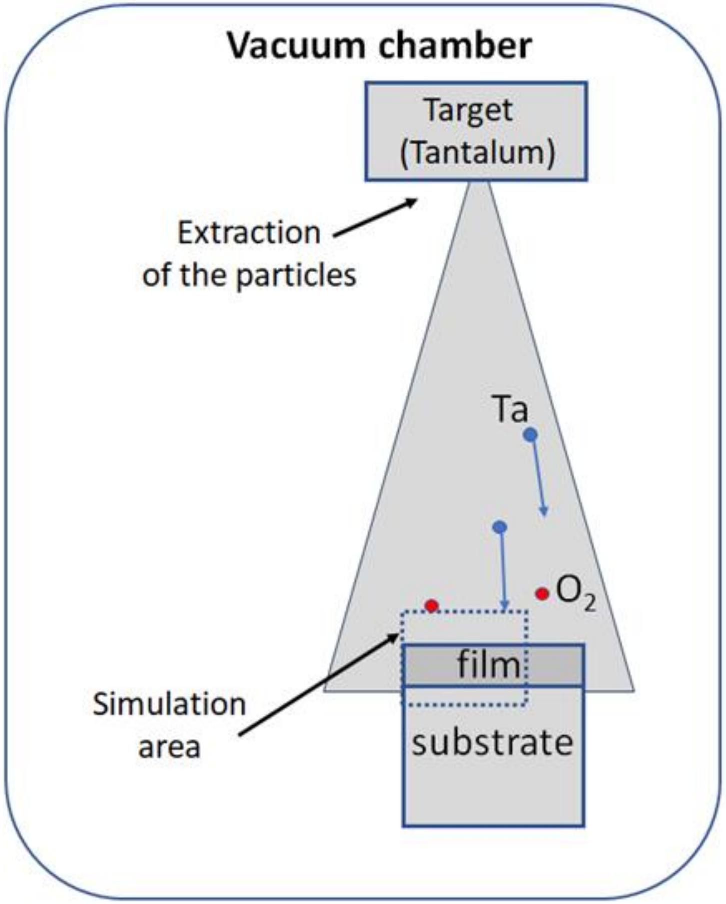
Цели моделирования:

1. Разработка методов математического моделирования процесса напыления тонких пленок, ориентированных на использование технологий суперкомпьютерных вычислений.
2. Разработка численных методов расчета структурных и механических свойств тонких пленок с использованием атомистических кластеров, полученных в результате моделирования процессов напыления. Программная реализация разработанных методов.
3. Исследование зависимостей структурных и механических свойств тонких пленок от технологических параметров процесса напыления.

Просветление оптики



Напыление пленок. Метод моделирования



$$m_i \frac{\partial^2 \vec{r}_i}{\partial t^2} = \vec{F}_i, \quad \vec{F}_i = -\frac{\partial V}{\partial \vec{r}_i}, \quad V = V(\vec{r}_1, \vec{r}_2, ..., \vec{r}_N)$$

Classical MD simulation:

force field, periodic boundary condition, thermodynamic ensembles - NPT (constant number of particles, pressure and temperature), NVT constant number of particles, volume and temperature)

$$U = q_i q_j / r_{ij} + A_{ij} / r_{ij}^{12} - B_{ij} / r_{ij}^{6}$$

Interaction	A_{ij} (kJ·nm^{12}/mol)	B_{ij}(kJ·nm^6/mol)
Ta-Ta	$3.12 \cdot 10^{-8}$	0
O-O	$2.5 \cdot 10^{-6}$	0
Ta-O	$4.5 \cdot 10^{-7}$	$1.0 \cdot 10^{-3}$

The goal of simulation: to achieve an understanding of influence of fabrication parameters on the properties of films in the scale of ~10-100 nm

Почему Ta2O5? Низкая шероховатость, аморфная структура

Chun Guo et al, Opt. Continuum **3**, 1679-1687 (2024)

Ta_2O_5: optical coatings in near-UV (300 nm) to IR (10μm) spectral range owing to its high chemical, thermal, and mechanical stability, high refractive index and high transparency; used in high-power lasers, gravitational wave detection, optical communication, and space optical systems, self-cleaning coatings.

e-beam evaporation with plasma ion-assisted deposition, 120 C

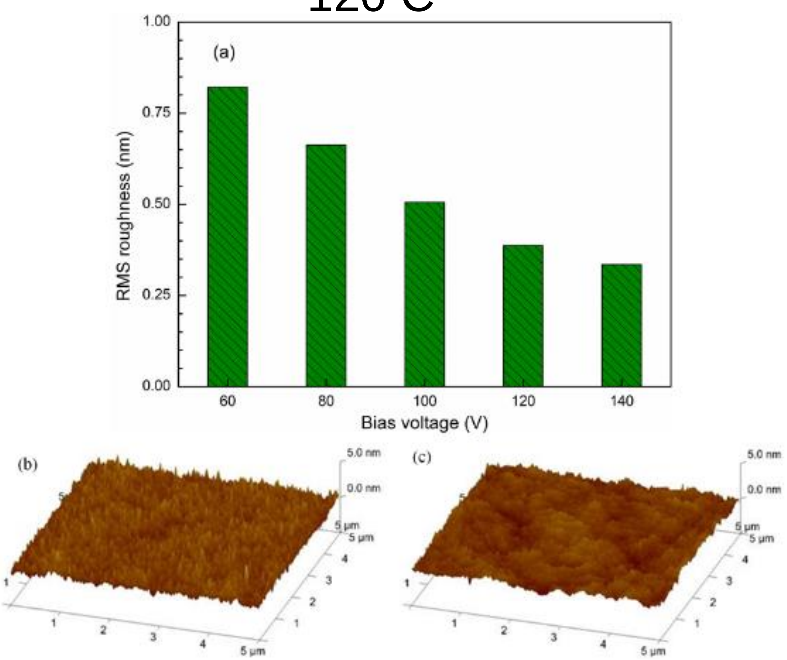
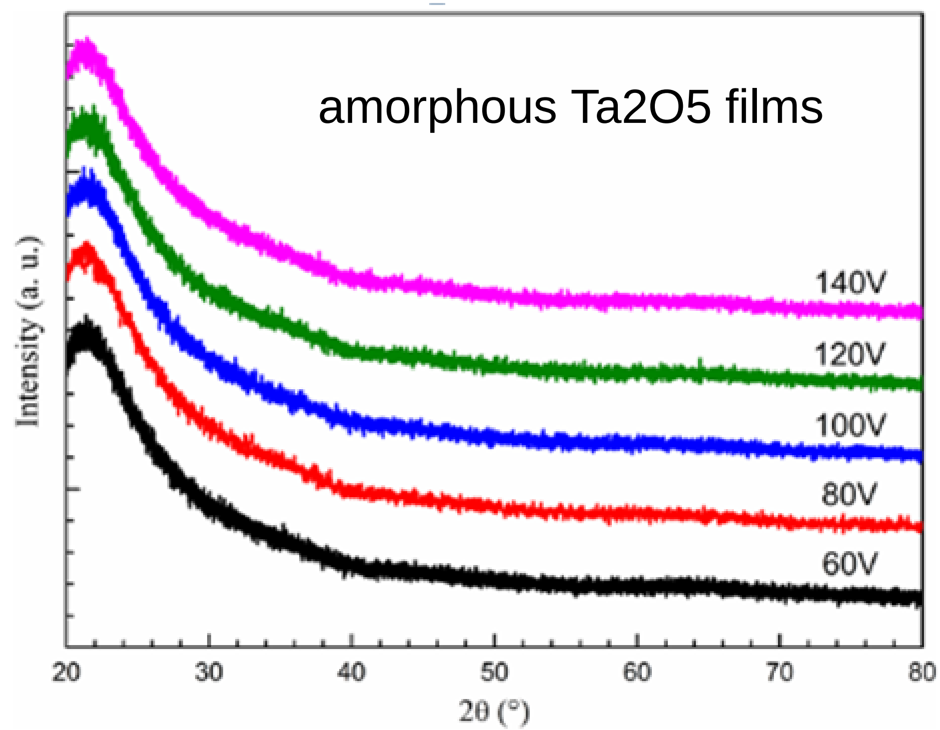
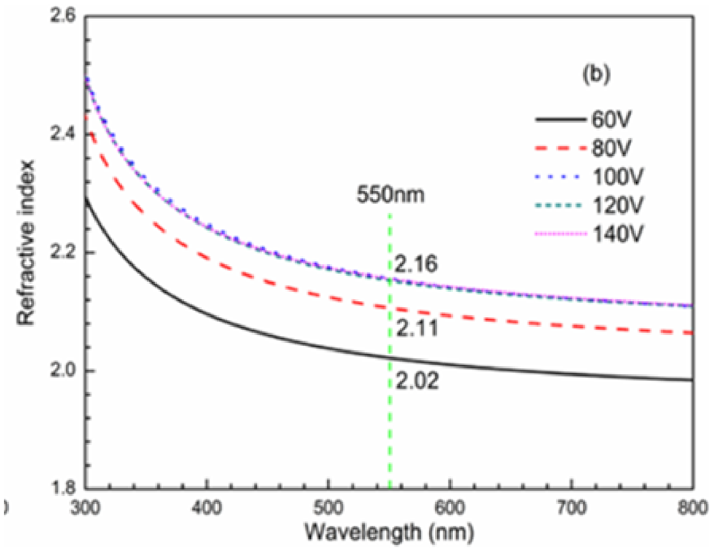


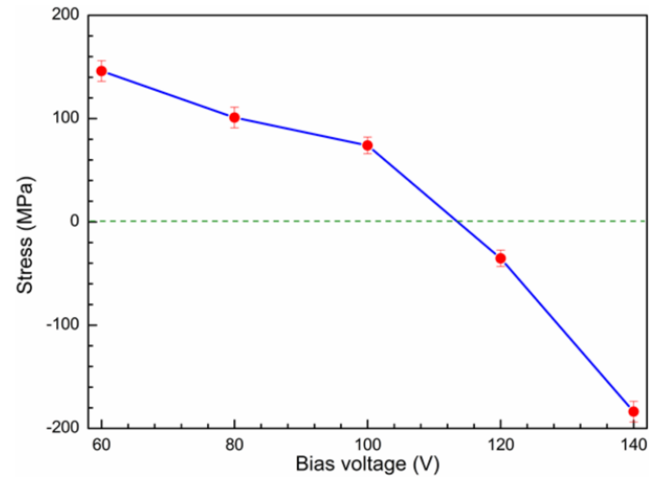
Fig. 4. (a) RMS roughness of PIAD prepared Ta_2O_5 film as a function of APS bias voltage. 3D surface topography of Ta_2O_5 films deposited with an APS bias voltage of (b) 80 V and (c) 120 V, respectively.

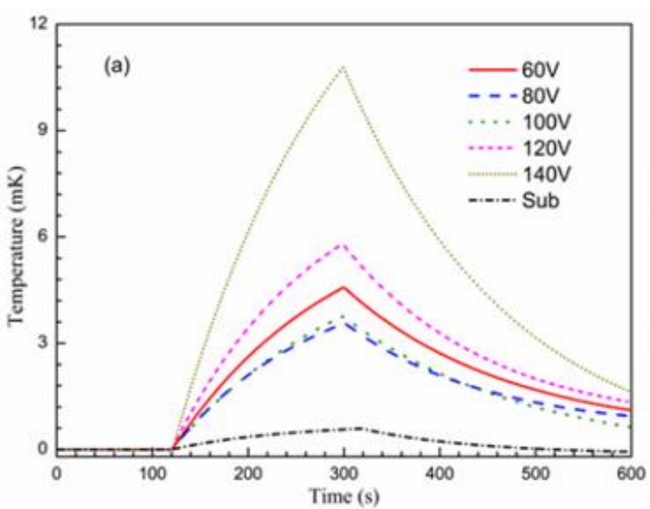


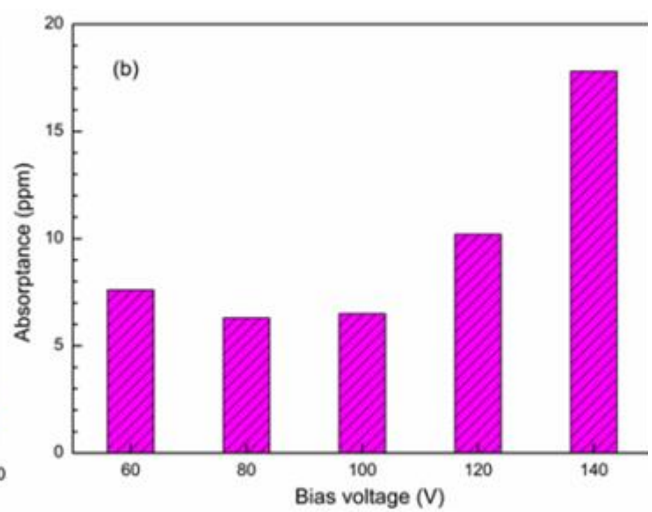
Ta_2O_5: показатель преломления, напряжения, поглощение

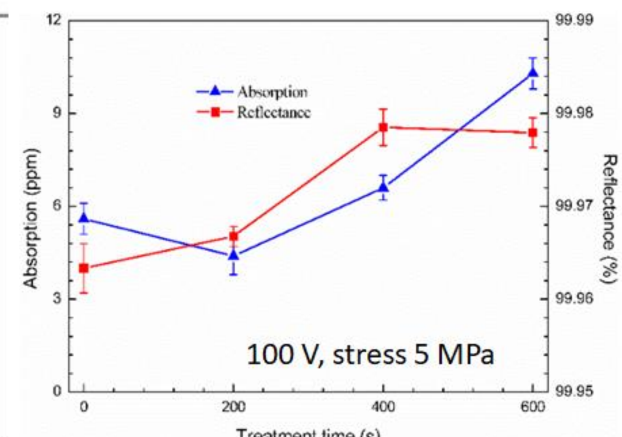
Chun Guo et al, Opt. Continuum **3**, 1679-1687 (2024)





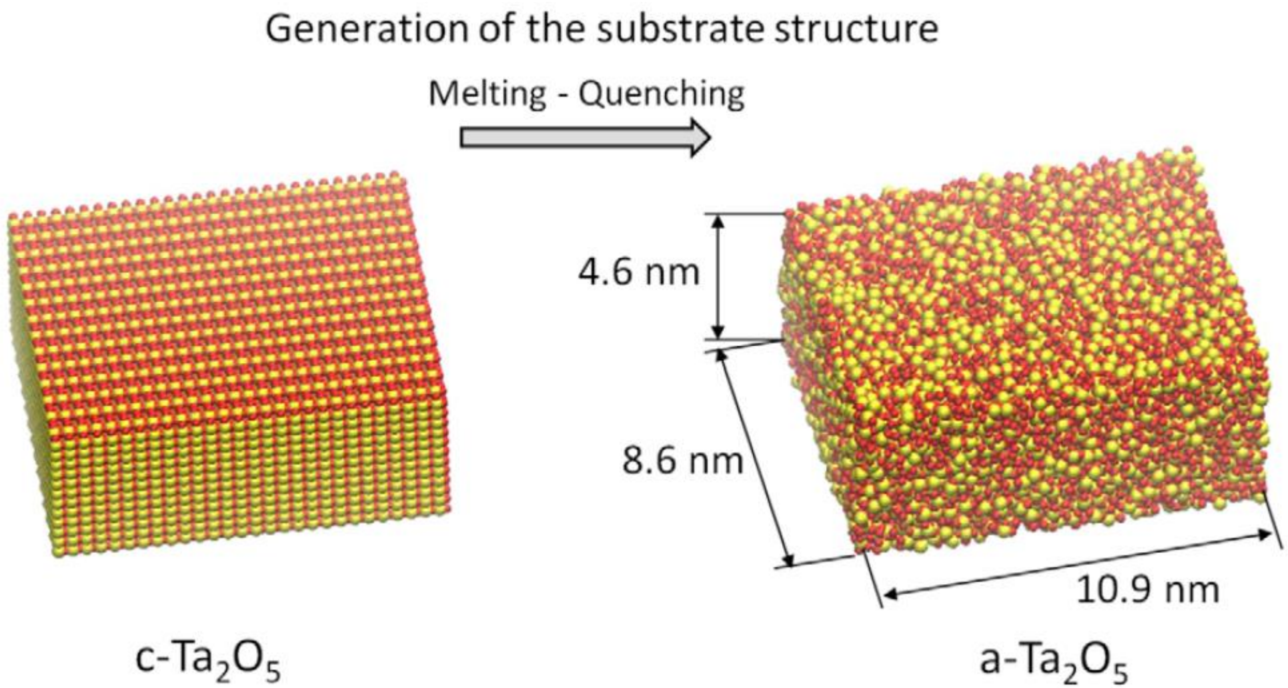






1064 nm high reflective (HR) coating consisting of Ta_2O_5 and SiO_2

Создание подложки



1. Heating from room temperature to $5 \cdot 10^3$ K during 500 ps;
2. Simulation of the structure at $5 \cdot 10^3$ K during 1 ns;
3. Cooling from $5 \cdot 10^3$ K to room temperature during 500 ps;
4. Equilibration of the obtain structure during 100 ps.

Радиальная функция распределения a-Ta_2O_5

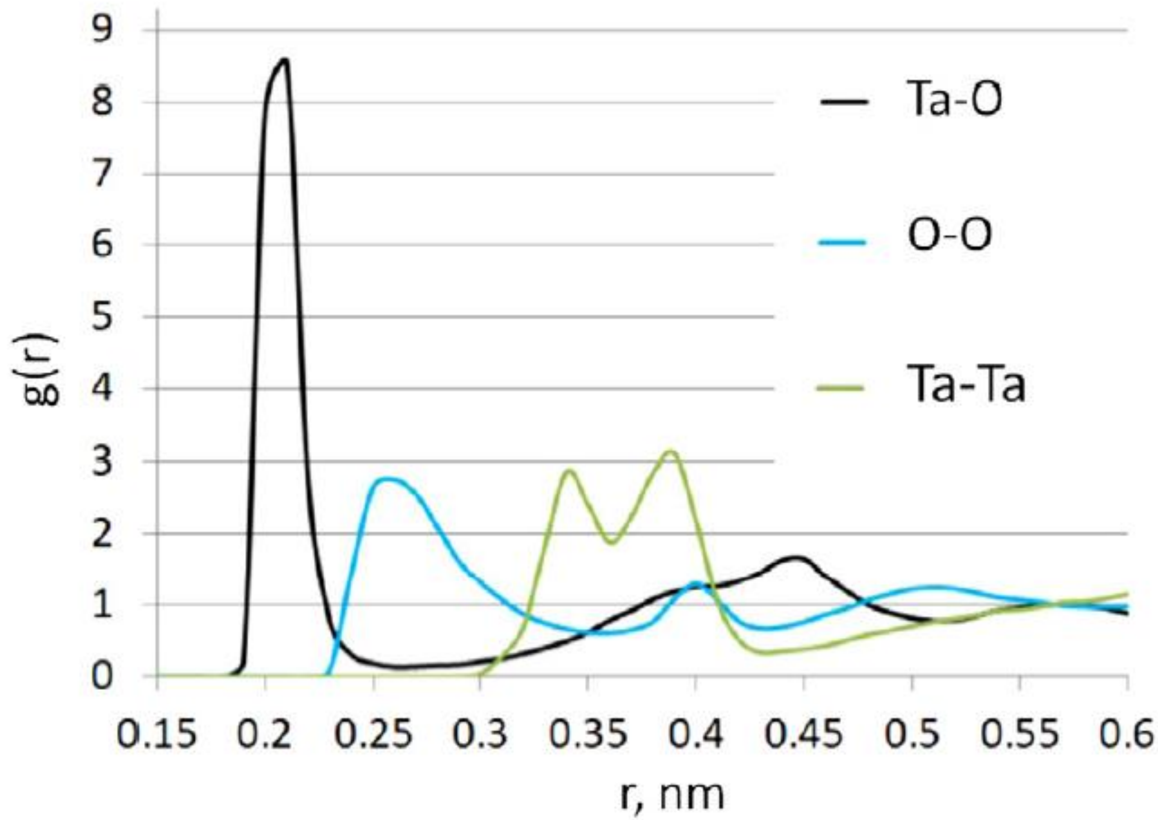


Fig. 3. Radial distribution functions of the amorphous Ta_2O_5; results of the MD simulation.

F. V. Grigoriev, V. B. Sulimov, D. C. Kutov, and A. V. Tikhonravov, "Structural properties of Ta_2O_5 deposited films using atomistic modeling," Appl. Opt. **64**, 369-376 (2025)

Профили плотности пленок a-Ta_2O_5

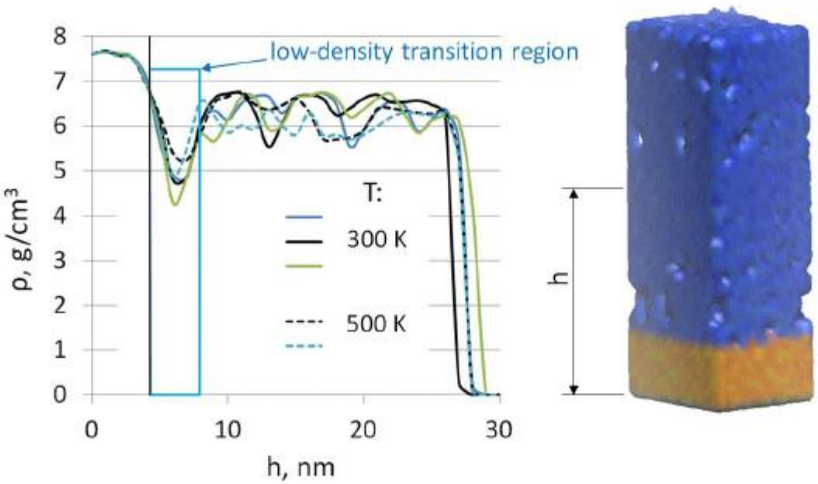


Fig. 5. Density profiles of the low-energy deposited Ta_2O_5 films; results of the MD simulation, E(Ta) = 0.1 eV; T is the substrate temperature. The profiles differ in the sets of random numbers used to specify the initial coordinates of the deposited atoms. The vertical black line marks the boundary of the substrate.

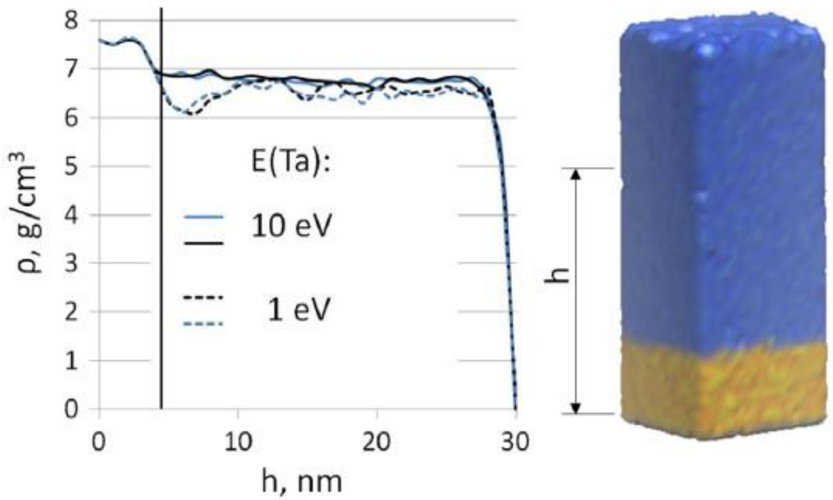
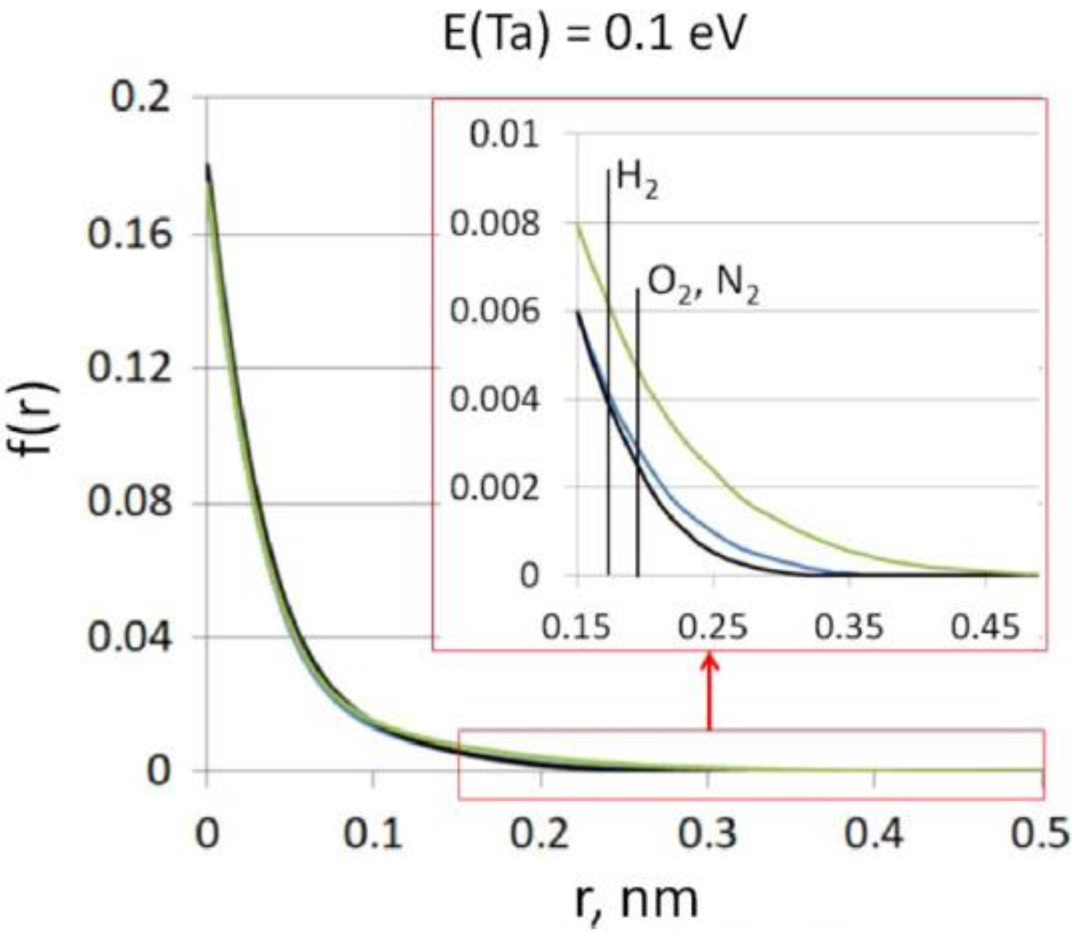
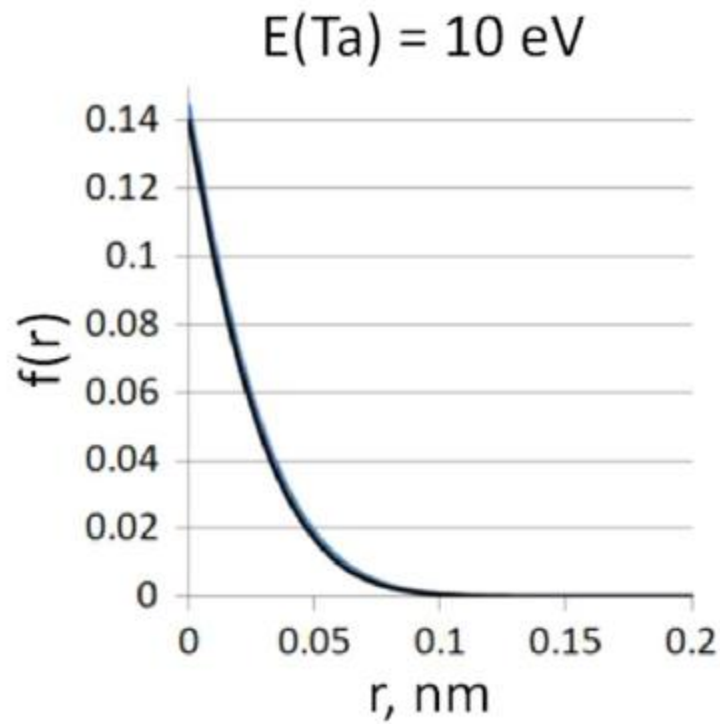


Fig. 6. Density profiles of high-energy deposited Ta_2O_5 films for two values of deposited Ta atom energies; MD simulation results. The substrate temperature is equal to 300 K. For each energy value, two profiles are shown, differing in the sets of random numbers used to specify the initial coordinates of the deposited atoms. The vertical black line marks the boundary of the substrate.

Пористость напыленных пленок



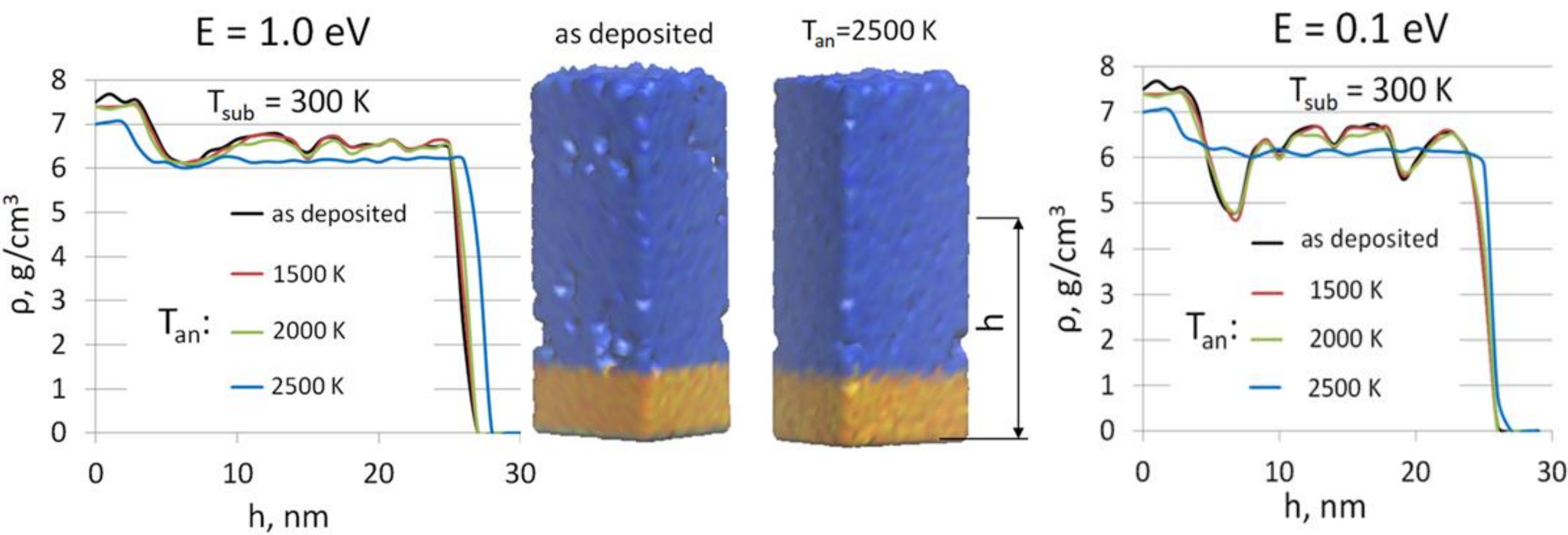


Pore distribution function for deposited films

Моделирование отжига. Профили плотности

Annealing of the deposited films begins after the deposition is completed. The annealing simulation consists of the following steps:

1. Heating of the deposited film cluster from the room temperature 300 K to the value T_{an}. The temperature increases linearly over 300 ps;
2. MD simulation of the cluster at temperature T_{an} over 300 ps;
3. Cooling of the cluster from the T_{an} to room temperature. The temperature decreases linearly over 300 ps;



Влияние отжига на пористость пленок

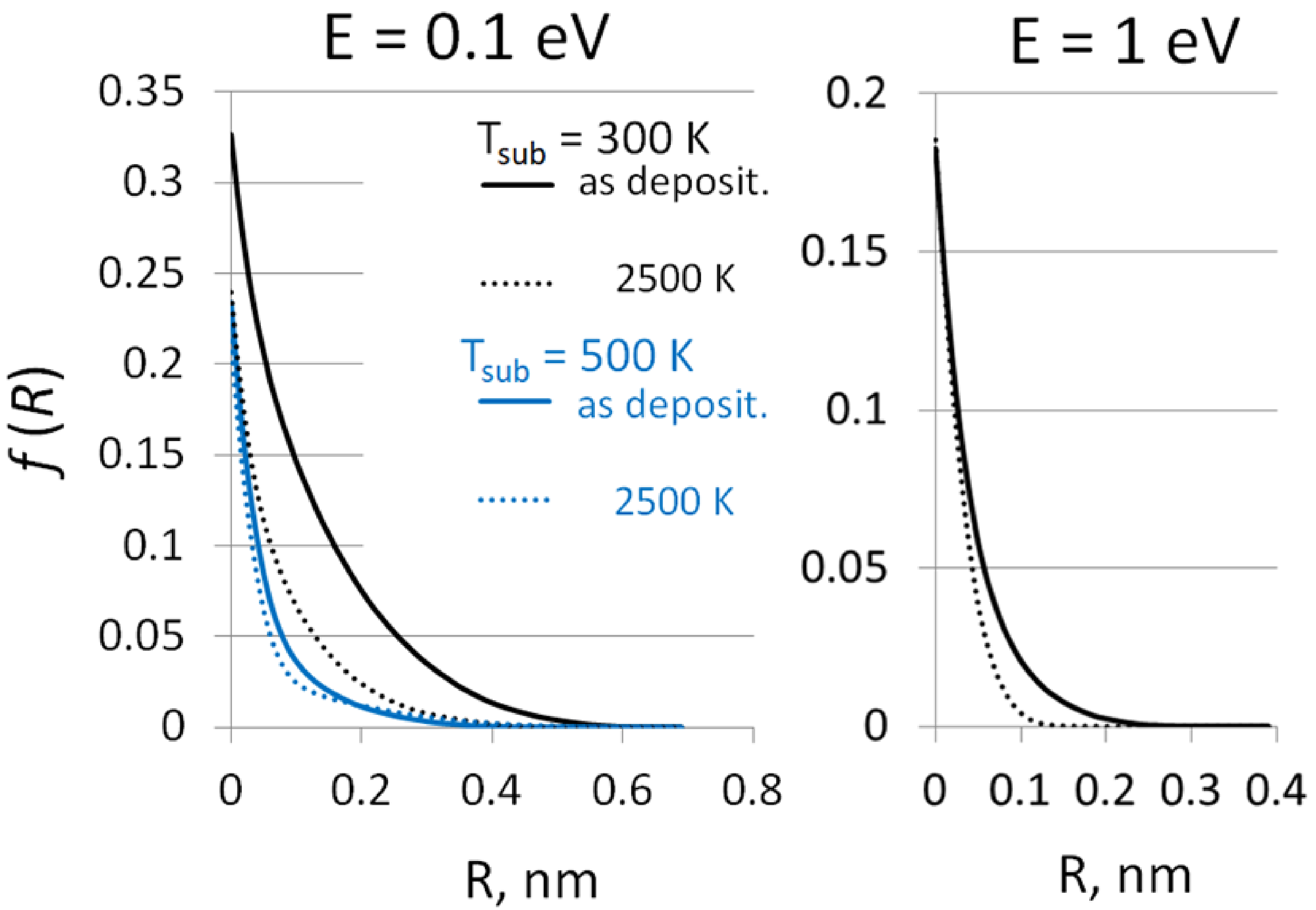


Fig. 3. Porosity of the "as deposited" and annealed Ta_2O_5 thin films; $f(R)$ is the pore distribution function, T_{sub} is the substrate temperature, E is the energy of deposited Ta atoms.

Координационные числа атомов в пленках

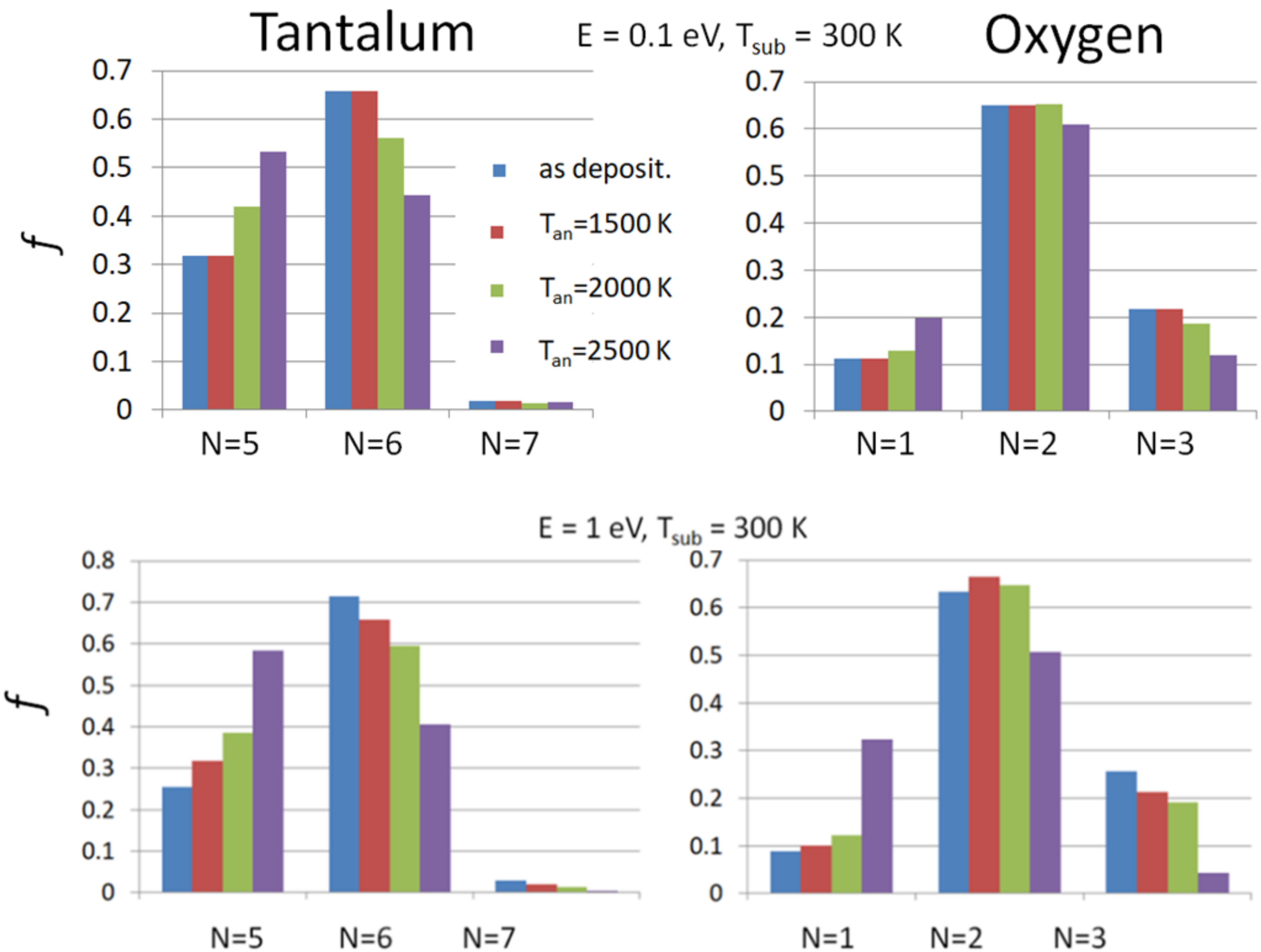


Fig. 4. Fractions of n-coordinated atoms of "as deposited" and annealed films, N is the coordination number, left and right sides show results for tantalum and oxygen atoms correspondently, T_{an} is the annealing temperature.

Численная эффективность моделирования

$$a = (t(N)/t(8))(8/N),$$

where t(8) and t(N) are the simulation times when 8 and N cores are used

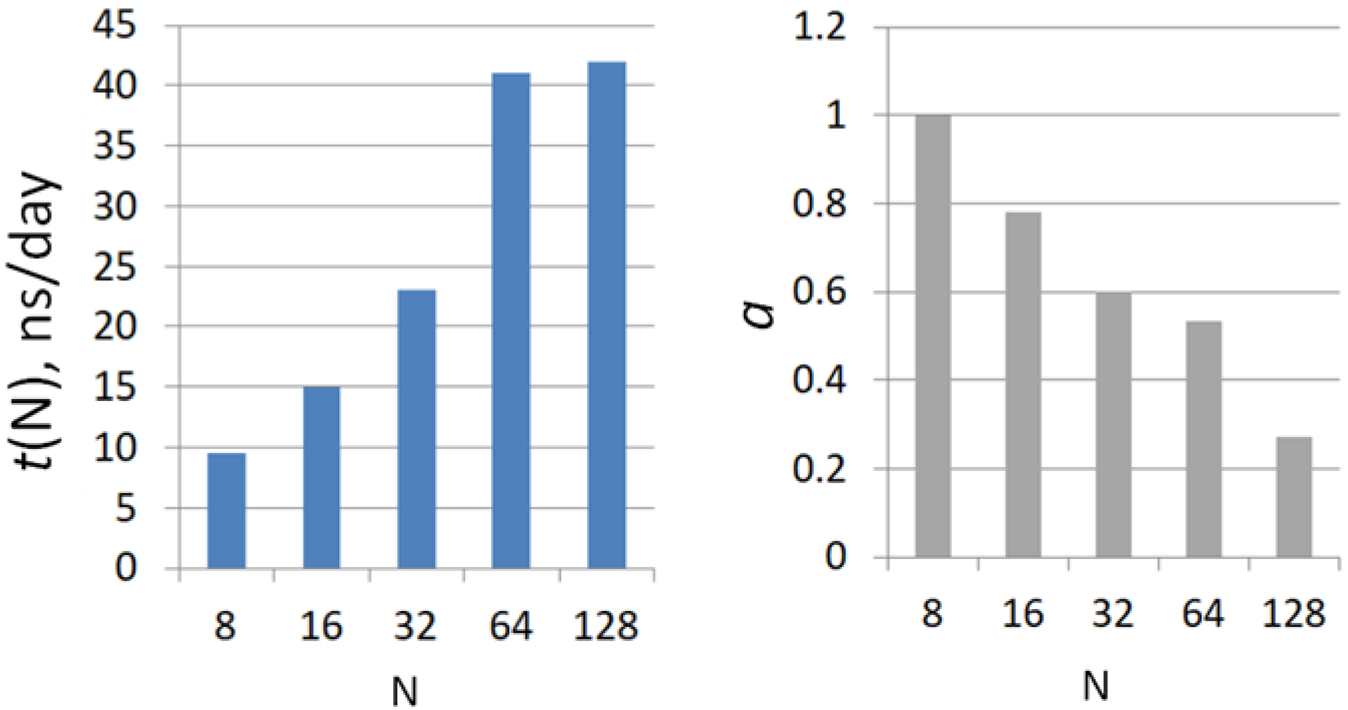


Fig. 5. Dependencies of the length of the MD trajectory (left side) and efficiency of parallel computations, *a* (Eq. (3), on the number of cores N.

Заключение

1. Annealing at relatively low temperatures does not have a noticeable effect on the density profiles of the films. **Increase in the annealing temperature results in smoothing of density profiles,** including the low density region between the substrate and the films.
2. **The porosity of film deposited on cold substrate at low energy of incoming Ta atoms reduces significantly**, especially for the pores with characteristic dimension more than 0.4 nm. **Thus, annealing affects the ability of Ta_2O_5 films to absorb molecules from the atmosphere**.
3. Annealing changes the distribution of atoms by coordination number: **the fractions of five-coordinated Ta atoms and one-coordinated oxygen atoms grows,** the fractions of six-coordinated Ta atoms and three-coordinated oxygen atoms reduces.
4. **Using of GPU accelerates calculations by three to five times.** The efficiency remains relatively high when the number of cores does not exceed 64, but then sharply reduces.

Спасибо за внимание!