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Computer simulation studies of roughness of thin films formed in the ion beam assisted deposition (IBAD) process

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In this study we present Monte Carlo simulation studies of thin films deposited in the ion beam assisted deposition (IBAD) process. The simulations were performed on a simple cubic lattice with the Metropolis sampling algorithm. Examination of the microstructure and morphology of the simulated film shows that the processes of the surface diffusion of adatoms and the sputtering of the film during its growth as a result of the ion bombardment significantly influence the structure of the deposited layer. The presented simulation model enables one to determine the importance and the influence of these processes on the final structure of the film.

Keywords: Monte Carlo simulation, ion beam assisted deposition (IBAD), thin films growth, morphology, roughness.

1. Introduction

The development of methods of deposition from the gas phase (PVD), in which the source of ions is a partially ionized gas, excitation plasma or a ion beam (IBAD) enables one to employ the ions as a kind of nano-devices in a material science [1, 2]. The contemporary microelectronics, micromechanics as well as the optoelectronics require the use of layers deposited in low-temperature processes. The layers with a good adhesion should have a well defined nano-structure and the topography described by means of the roughness parameter or a fractal dimension [3–5]. The use of the ion bombardment in the deposition process enables one to meet these technological requirements. This is confirmed by experimental results published in recent years [6–9]. Thanks to better understanding of the processes of the layer growth (in an atomic scale) as well as the statistical description of these phenomena, the computer simulations can be applied [10, 11]. The simulation results enable one to inspect the microscopic scale of the deposition and to manipulate the parameters of the process

in order to achieve the required results. Atomistic computer simulations become increasingly helpful in understanding the nanoscale processes that are essential in thin film formation and ion-beam modification [12]. In addition, the computer simulations provide a very useful tool for visualizing as well as testing atomistic models of film growth [13–17]. The simulation results are useful in prediction of the properties of deposited layers and can serve as a flexible tool in preparation of real experiments.

In our previous Monte Carlo simulation studies of the film growth in the IBAD process we investigated the influence of ion beam energy (E_i), the ion-to-atom arrival ratio (IAR) value, angle of ion beam incidence α and the temperature T of the substrate on the properties of the obtained layer, namely the surface roughness [18–21]. In this paper we focus our attention on the role of the adatom–adatom and ion–adatom interactions as well as the energy of the deposited atoms on the film growth. The aim of this study is to find these parameters of the process which are the most important from the point of view of the properties of the film.

2. Model

We developed a ballistic Monte Carlo model of an IBAD deposition process. In our model we focused on the following elements: atoms, ions, adatoms and the substrate surface. All the elements of the model were located in the lattice sites (knots) of the simple cubic lattice. At the beginning of the simulation the substrate had a randomly computer-generated surface (about 5 monolayers thick), what simulated an initial substrate roughness. We assumed that the atoms arrived to the surface following the trajectory which was perpendicular to the *xy* plane. The arrival of the ions took place by the linear trajectory which formed an angle α to the normal.

In order to control the proper interactions between the particles represented in the model, we assumed kinetic energies of the particles as well as the interactions between them at the temperature of the substrate T. All these parameters are in arbitrary units. The kinetic energy was associated with both the atoms (E_a) and the ions (E_i). We assumed that the energy values of ions and atoms did not change during their arrival to the surface. After the deposition of a particle on the substrate this energy was dissipated between the neighboring particles at equal parts. The IAR defined as the number of ions in a ion beam to the number of adatoms arriving to the substrate was also the parameter of the model. The scheme of the model is presented in Fig. 1.

The values of the kinetic energy were set arbitrarily, however the energy of the ions was much larger than that of atoms. All the values of energy in the model had a Gaussian distribution (the values given in the simulation data were the ensemble averages).

The adatom arriving to the surface interacted with the already deposited material in the following way:

– an arriving adatom (or an ion) could transfer its kinetic energy (namely, its component parallel to the surface) to the particle neighboring its final location on

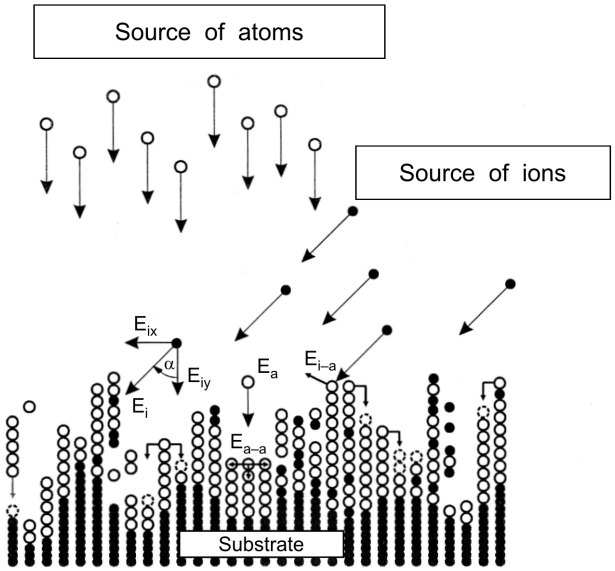

Fig. 1. Scheme of the model.

the surface in the process of the elastic collision. The effect of such collision would be the move (one lattice site ahead) of the particle, if a new position were not occupied. This mechanism resembles the lateral solid-state diffusion;

– an arriving particle could transfer its kinetic energy (namely, its component perpendicular to the surface) to the particles located on the surface of one lattice site below its "landing" site. The result of such energy transfer is the possibility of moving some surface particles down into the layer – this is called a "pinning" effect;

– an arriving ion could transfer its kinetic energy to the already deposited material, then the sputtering of that material could take place.

All the above mentioned rearrangements of the particles in the growing layer were the subjects to the acceptance based on the total balance of the energy of the system "before" and "after" the proposed change according to the Metropolis scheme [22, 23]. The total balance of the energy of particles was done taking under consideration the following interactions: ion–adatom interactions $E_{\mathrm{i-a}}$, adatom–adatom interactions $E_{\mathrm{a-a}}$, and ion–ion interaction energy was assumed to be zero as the state of reference. The rearrangements of the particles were then accepted with the probability proportional to the Boltzmann factor $\exp(-\Delta E/k_B T)$. Here ΔE was the gain of the particle energy after the collision and T was the temperature of the substrate. If the total energy of the system were lower after the modification, the new positions of particles would be accepted unconditionally.

The preliminary verification of the model with the experiment has been done – the roughness of CrN layer with the energy of ion beam was measured. The results were presented in [24].

3. Results and discussions

The aim of this work was to determine the influence of the internal interactions and relaxation phenomena on the morphology and the topography of the surface in the proposed ballistic model of the IBAD enhanced deposition. All other parameters of the process were taken as constant – their influence on the simulation results was investigated previously. We have performed a series of simulations with variable input parameters such as: E_i, E_a, E_{a-a}, E_{i-a}, T and IAR. In all simulations we obtained the computer-generated layer on the substrate with a pronounced columnar structure and some number of empty sites inside them. As an example of such layer we show the cross sections for two different values of ion energy (all other parameters remained constant) – see Fig. 2. One can observe the differences in the layers' thickness as well

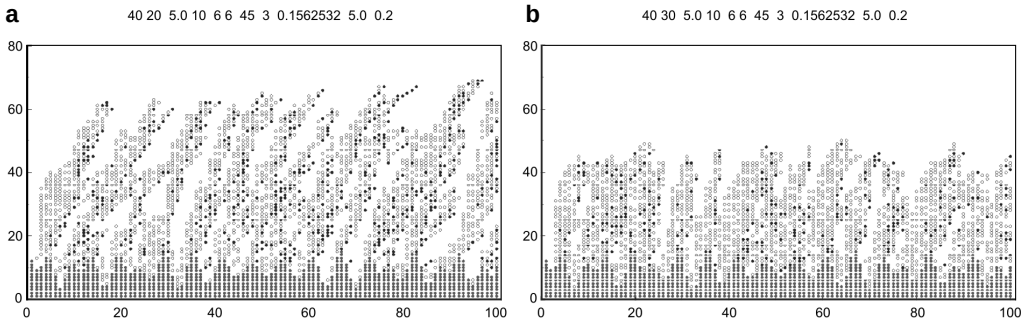

Fig. 2. Cross-section profiles of the simulated films at various ion beam energy E_i: E_i = 20 (**a**) and E_i = 30 (**b**). For all figures E_a = 5.0, E_{a-a} = 10.0, E_{i-a} = 6.0, T = 6.0, α = 45°, IAR = 5.0. Black circles represent ions and open circles represent adatoms. The profile of the substrate was simulated. The x and y axis values are given in lattice units.

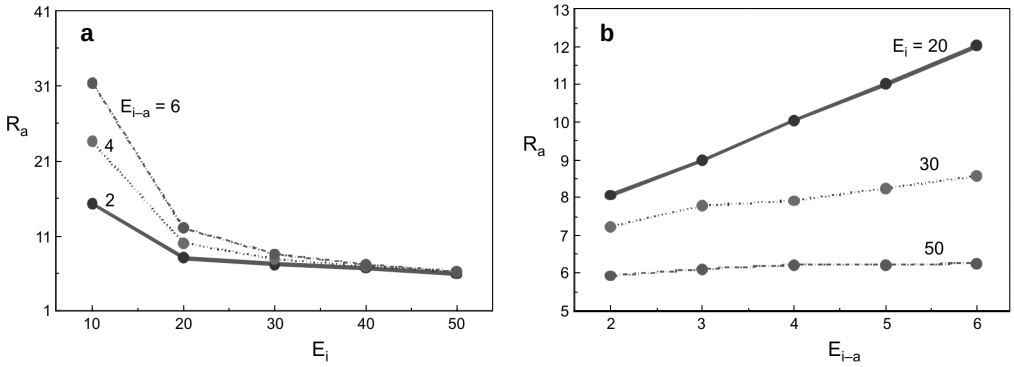

Fig. 3. Dependence of the roughness R_a (in number of monolayers) of the simulated films *vs*. the ion beam energy E_i (**a**) for different ion–adatom interaction energy E_{i-a} and *vs*. ion–adatom interaction energy E_{i-a} (**b**) for different ion beam energy E_i at E_a = 5.0, E_{a-a} = 10.0, α = 45°, T = 4.0, IAR = 3.0. Temperature T is given in arbitrary units.

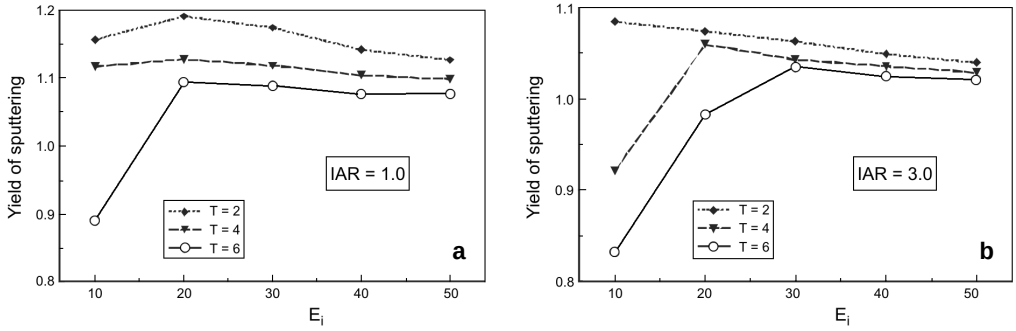

Fig. 4. Plots showing the yield of sputtering for different IAR values IAR = 1 (**a**) and IAR = 3 (**b**) as a function of the ion energy E_i. The appropriate values of temperature T are given in the legend.

as in their structure – the lower ion energy gives more fibrous structure of the layer. Also the densification of the layer for the larger ion energy is visible. This is a result of more intensive effects, such as pinning effect, sputtering and rearrangement processes.

The quality of the deposited film is usually characterized by the roughness parameter R_a. The dependence of R_a (in lattice units) of the layer on the kinetic energy of ions E_i and the energy of ion–atom interaction parameter E_{i-a} are presented in Fig. 3**a**, **b**, respectively. The roughness parameter was calculated according to the well known formula $R_a = \left|\overline{h - \bar{h}}\right|$, where h is the local height of the layer and the dash denotes mean values. The values of ion–atom interactions influence strongly the roughness of the layer, especially for low values of the ion kinetic energy E_i. For high values of E_i the ion–atom interactions have less meaning, and the morphology and the topography of the layer almost do not depend on it.

Analyzing the optical quality of the sample, one can ask the question: what is the most important mechanism which decides on the structure and the roughness of the film in the low energy regime? First, we investigated the sputtering of atoms deposited in a layer in the IBAD process. We calculated the ratio of the number of sputtered atoms to the number of ions – a yield of sputtering. In Fig. 4 we present the plots showing the yield of the sputtering for the cases of IAR = 1 and 3 as a function of the ion energy E_i. The calculations were performed for different substrate temperatures T. One can notice that for high values of ion kinetic energy E_i the sputtering yield remains almost constant. However, it is interesting that for low energies E_i the increase in the IAR gives the same sputtering yield as the increase in the temperature T. The analysis of the pinning process is shown in Fig. 5. The plots show the fraction of the successful attempts of pinning the adatoms in the deposited layer. Here one also observes that the energy of ions strongly influenced the efficiency of the pinning. However, at high values E_i, the process almost did not depend on it. The changes in IAR almost did not change the pinning effectiveness. From the presented results we can conclude that there exists a threshold energy – the processes below this value express the sensitivity to the parameters that change the roughness of the sample. Therefore, in this parameter

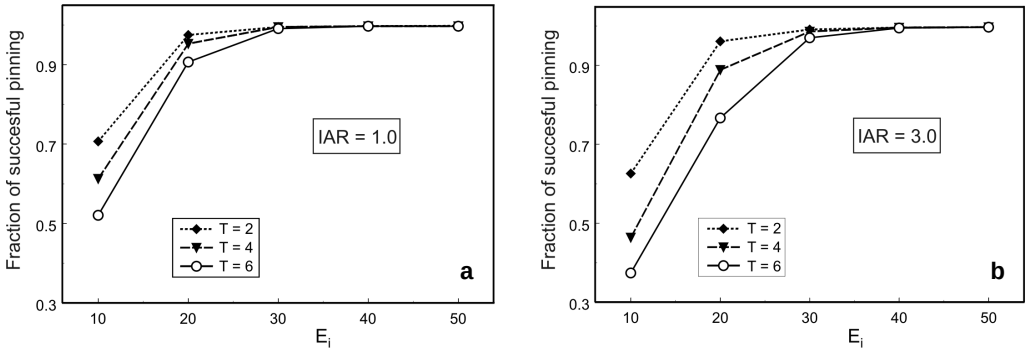

Fig. 5. Plots of the fraction of successful pinning for different IAR values IAR = 1 (**a**) and IAR = 3 (**b**) as a function of the ion energy E_i. The appropriate values of temperature T are given in the legend.

region one can control the deposition in order to obtain the required properties of the layer.

Taking the complexity of the simulated process into account, one has to realize that the course of the simulation depends on many input data and it is difficult to find simple dependences between the parameters of the deposition process and the characterization of the obtained layers. The conclusions that we can present now are that the energy of the ions and the ion–adatom interactions play a substantial role in the determination of the properties, mainly the roughness of the layers obtained in the IBAD process. The increase in the energy of the ion beam leads to the reduction of the roughness of the layer as well as to the increase in the film's density, what is essential for a good optical quality of the layer.

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