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Growth of the optical layers in a stochastic simulation. Study of a film morphology

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A Monte Carlo simulation model of the ion-beam assisted deposition (IBAD) process was used to investigate the influence of some process parameters on the final quality of thin films. The simulations were performed on a simple cubic lattice on which the particles were located. The results show that the angle of ion beam incidence, as well as the kinetic energy of particles, ion-to-atom arrival ratio (IAR) and the roughness of the substrate play an important role in the quality of the obtained films. The influence of the deposition process parameters on the morphology of the films was also discussed.

1. Introduction

In recent years, thin film deposition in the presence of an ion beam generated from ion source (IBAD) has focused the attention of researches interested in hard, wear resistant and optical coating fabrication [1] – [5]. In many cases the optical layers of an exceptionally high quality are needed. In particular, the layers should have a low (or alternatively high) level of optical absorption and the coefficient of refraction of the layer material should be independent of the layer thickness. The layer interface should be as smooth as possible (to reduce the light dispersion) and the properties of the layer in changing ambient conditions (moisture, temperature) should be constant. The layer should adhere to the substrate, be hard enough and resistant to wearing. The fulfilment of such demands becomes possible when the employed technological methods ensure precise control of deposition process parameters and when the correlation of the parameters with the layer properties is known.

Among the numerous methods of layer deposition the dynamic ones enhanced with ion beam bombardment ensure the highest precision of parameter control. The IBAD process is a combination of two distinct physical processes: an ordinary physical vapour deposition on biased or unbiased substrate and a simultaneous bombardment of the surface with low-energy ion beam [6]. The main parameters of this method are: the ion beam energy (current), the rate of material sputtered from target in direct current process, the ion-to-atom arrival ratio (IAR) and the angle of ion beam incidence (with respect to the normal). The initial substrate temperature and ion bombardment influence the nucleation conditions and the kinetics of the layer growth (physical mixing enhanced diffusion), as well as the final structure (morphological and crystallographic changes), and modifies the physical properties of the layers (adhesion) [7].

Technological progress in designing complex optical systems, widely applied in laser technique or in optical components of the classical optical designs, depends to a great extent on the recognition and understanding of the layer growth process and its effect on microstructure and topography of their surfaces. The surface is described by the roughness, which can be measured in a relatively simple way and correlated with the optical properties of the layer.

Many authors have used simulation techniques (molecular dynamics and Monte Carlo methods) for atomistic modelling of the processes occurring during the growth of the layers [8]–[10]. Here we present the continuation of our previous work on the growth of films (including the pinning effect) deposited in the IBAD process on the substrate which can have a distinct profile in the initial stages of the process.

2. Model

A detailed description of the Monte Carlo model of the IBAD growth process has been presented in our previous papers [11], [12], therefore here the assumptions of the model are briefly described. The model involves a square surface substrate of 100 by 100 lattice units, *i.e.*, there are 10^4 lattice points in which the arriving particles can be deposited. The adatoms, as well as arriving ions, can be located in lattice points only. The model uses a simple cubic lattice what makes the idea simple and speeds

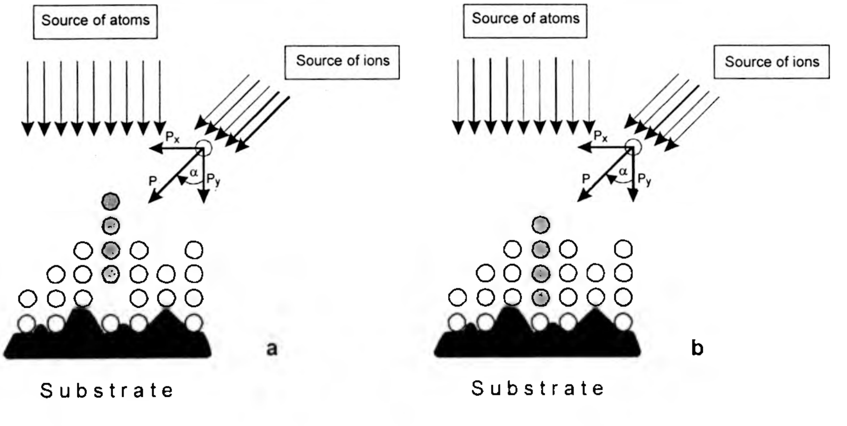

Fig. 1. Scheme of the model (including the pinning effect and roughness of the substrate): **a** – before pinning effect, **b** – after pinning effect. Adatoms marked as gray are the subjects to the "pinning" effect, when bombarded by ions from Kaufman source. The grey column of adatoms is moved towards the bottom of the substrate layer. Vector **P** denotes the momentum of the ion.

up the calculations. Moreover the lattice approximation is reasonable in the solid state thin films. The beam of atoms (originating from a Kaufman source) of deposited material is perpendicular to the layer of substrate on which the deposition takes place. The process of the deposition of material atoms is accompanied by a beam of ions, which arrive at a certain angle with respect to the normal as is shown in Fig. 1.

In order to determine the influence of the parameters of the process on the final quality of the optical film a series of simulations were performed by varying the process conditions and then checking the properties of the layer, such as its topography, roughness and thickness. All particles arrive onto the substrate along linear trajectories. During the deposition process an interaction between the growing film (consisting of adatoms and ions) and the arriving particles (atoms and ions) takes place. It was assumed that the arriving particles have certain kinetic energy which can be exchanged in an elastic collision energy transfer process. We also assumed that the ratio of the kinetic energy of the ions to the kinetic energy of the atoms arriving onto the substrate is 100. In order to avoid local overheating of the system in our model 20% of the energy is dissipated during each cycle of the process. For all elementary processes which were accompanied by the changes of the energy of the system due to creation of new interactions (or breaking old ones), the sampling Metropolis criterion was applied: the process that leads to the growth of the energy of the system is weighted by a Boltzmann factor: $\exp(-\Delta E/k_B T)$, where ΔE is the total change of the energy of the system in the given elementary process, k_B is the Boltzmann constant and T is the temperature of the system; in arbitrary units). The mass transfer was also introduced into the model according to some simple mechanisms: particle motion along the layer of the film and vertical motion of the clusters of adatoms caused by the beam of ions (pinning effect).

3. Results and discussion

The main aim of this work was to examine the influence of simulation parameters on topography, roughness and thickness of the obtained layers. In the computer simulation program one of the geometrical structure factors of the substrate, which is very important for the layer growth, is its roughness. Therefore, the roughness was analysed in detail. Computer simulated profile of surface roughness was characterized by means of the following parameters (given in lattice units): mean square deviation of the profile from the mean line R_q and the parameter describing the longitudinal features of the profile, *i.e.*, the average distance of roughness S_m [13]. The layer growth on the substrates with diverse features of surface roughness was simulated for flat, "random" ($R_q = 2.43$ and $S_m = 6.57$) and "sinusoidal" ($R_q = 2.06$ and $S_m = 4.40$) surface profiles.

An analysis of the performed simulations allows us to follow the process of the layers growth in the IBAD process and to evaluate the influence of the kinetic energy value of a deposited particle, the incidence angle of the ion beam, the ion-to-atom arrival ratio, as well as the influence of temperature and roughness of the substrate on the resulted homogeneity and roughness of the coating.

The results of the simulations are presented in two kinds of graphs: the cross -sections of the layer, which are perpendicular to the substrate surface – they give the idea on the morphology of the sample film. The plots show the functional dependences between some model parameters and the mean final results obtained during the simulations.

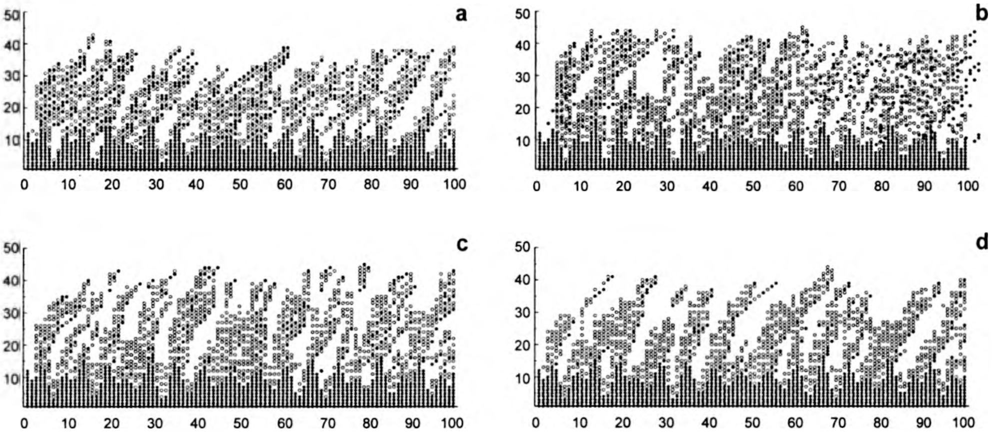

Fig. 2. Profiles of the simulated layers at various angles of the ion beam incidence α: 10° (**a**), 30° (**b**), 45° (**c**), 60° (**d**). For all figures $T = 4$, IAR = 3.0, R_q (substrate) = 2.43 (in lattice units).

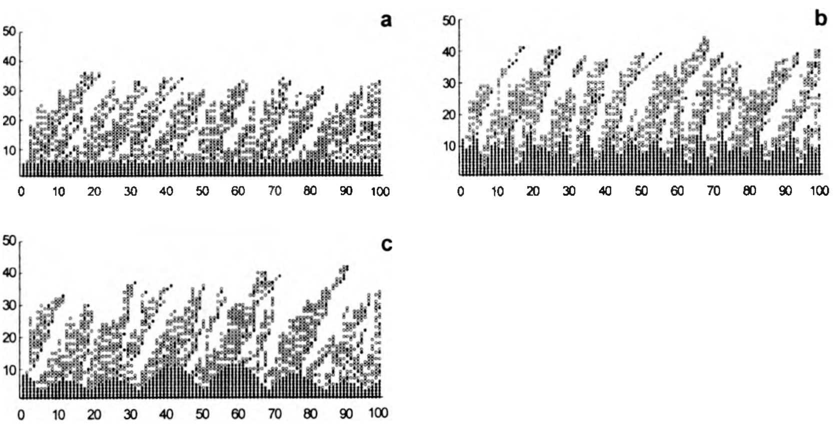

Fig. 3. Profiles of the simulated layers at various types and roughness of substrate: **a** – flat $R_q = 0$, **b** – random $R_q = 2.43$, **c** – sinusoidal $R_q = 2.06$ (in lattice units). For all figures $T = 4$, IAR = 3.0, R_q (substrate) = 2.43 (in lattice units).

The structure of the layers is shown in Figs. 2 and 3 where typical examples of the profiles are illustrated. Open circles represent adatoms, while filled dark circles represent ions. The profiles presented in Fig. 2 were obtained for different angles α

the ion beam incidence (all other parameters of the film growth simulation, *i.e.*, the IAR, the temperature of the substrate, the energy of the system and the roughness of the substrate were the same in all cases). The cross-sections of the layers reveal that the deposited layers form columnar structures the slopes of which are shifted towards the ion beam direction. Moreover, the increase of the angle α results in a more columnar structure of the layers and also leads to less built-in ions in the layers.

The roughness of the layer depends, to a large extent, on the profile of the substrate surface. In order to investigate the influence of the substrate characteristics we performed a series of simulations of film growth at the same conditions (the angle of ion beam incidence $\alpha = 60°$), however three different substrate profiles were used: one flat and two simulated with random and sinusoidal functions. The profiles in question did not change during the simulations of the IBAD process. Figure 3 presents the profiles of obtained layers. All examples show the columnar structure of the layers, but in the case of the random and sinusoidal substrates there is a strong correlation between the location (and the number) of columns and the structure of the substrate. The layers in the form of fibrous columns on "sharp" discontinuities of the substrate are the most probable to grow.

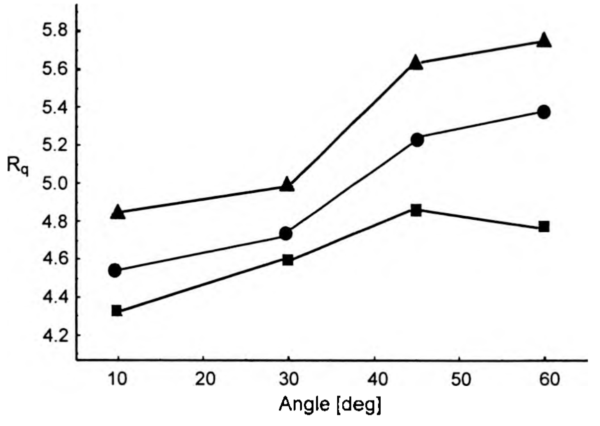

Fig. 4. Dependence of the roughness of the layer R_q on the angle of the ion beam incidence α for different cases of simulated profiles: ● — random, ▲ — sinusoidal, ■ — flat.

The roughness parameter R_q, which characterizes the optical quality of the film, is shown in Fig. 4 as a function of the angle α for different types of substrates. It may be seen that with the increase in the ion beam incidence angle α, there is a raise in the mean square standard deviation of the layer profile from the mean line R_q. This effect is more pronounced in the case of non-flat substrates for large values of angle α. Therefore, to improve the optical quality of the film one should perform the IBAD technique deposition at low angles of the ion beam.

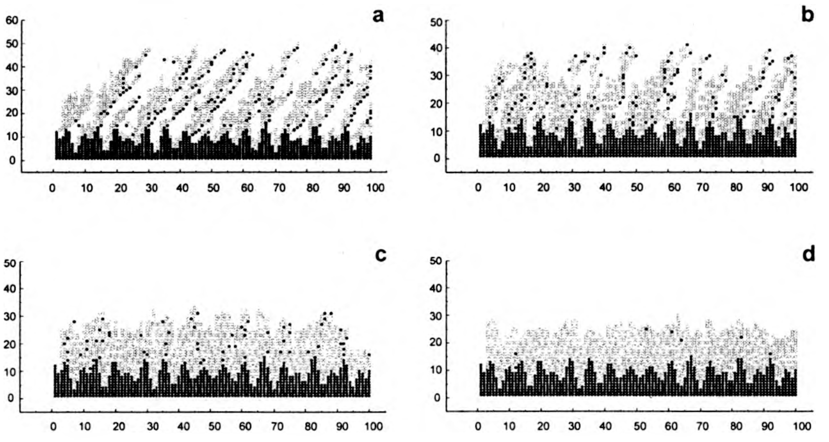

Fig. 5. Profiles of the simulated layers at various values of the ion beam energy E_i: 10 (**a**), 15 (**b**), 30 (**c**), 60 (**d**). For all figures $T = 6$, IAR = 3.0, $\alpha = 60°$, R_q (substrate) = 2.43 (in lattice units).

The series of profiles in Fig. 5 shows changes in the structure of layers along with changes in the ion beam energy E_i. Figure 5**a** presents the columnar growth of the layer with visible effect – all columns are oblique towards the ion beam direction. As the value of E_i increases the columnar structure of the layer disappears. The layer becomes more dense with smaller number of included ions. Also the effects of smoothening and thinning of the layer are observed. All these effects are due to the sputtering of the growing layer on the substrate by the high energy ion beam. This shows that the energy of the ion beam plays a very important, probably a crucial role in the layer growth process.

4. Conclusions

We have used Monte Carlo simulations to study bombardment of a growing film with ions in IBAD process. Ion bombardment provides the possibility to have condition for growing high quality films. Analysis of this work's results shows that:

– The effect the angle α magnitude of the ion beam incidence used in IBAD process on the morphology and, for example, on optical properties of thin layers. The increase in the incidence angle enhances the columnar growth of the layers and also leads to the lower number of built-in ions in the layers.

– The increase in the ion beam energy leads to smoother and thinner layers with fewer numbers of the induced ions.

– One can observe the influence of the substrate profile on final morphology of the deposited films. The final quality of the layer is the result of a multi -parameter process. Therefore, in order to understand the most important factors which determine the characteristics of the film, one can use such model and play with its parameters.

Such a game enables one to prepare the proper experiment which will verify the assumptions which were made in this simulation model.

References

[1] CEVRO M., CARTER G., Opt. Eng. **34** (1995), 596.

[2] OLESZKIEWICZ W., OLESZKIEWICZ E., ŻUKOWSKA K., Opto-Electron. Rev. **5** (1997), 133.

[3] OLESZKIEWICZ W., OLESZKIEWICZ E., ŻUKOWSKA K., Proc. SPIE **3820** (1999), 423.

[4] PULKER H.K., Surf. Coat. Technol. **112** (1999), 250.

[5] YASHAR P., BARNETT S.A., RECHNER J., SPROUL W.D., J. Vac. Sci. Technol. A **16** (1998), 2913.

[6] ENSINGER W., Nucl. Instr. Meth. Phys. Res. B **127/128** (1997), 796.

[7] ZDANOWSKI J., OLESZKIEWICZ W., Proc 12th International Special Summer School, *Modern Plasma Surface Technology*, Koszalin, Poland, 2000, p. 75.

[8] GILMER G.H., HUANG H., DIAZ DE LA RUBIA T., TORRE J.D., BAUMANN F., Thin Solid Films **365** (2000), 189.

[9] LUGSCHEIDER E., Von HAYN G., Surf. Coat. Techno.l **116-119** (1999), 568.

[10] MUELLER K.H., Phys. Rev. B **35** (1987), 7906.

[11] OLESZKIEWICZ W., ROMISZOWSKI P., Proc. VII Conf. *Electron Technology*, ELTE 2000, Polanica Zdrój, Poland, Institute of Microsystem Technology, Wrocław University of Technology, 2000, p. 950.

[12] OLESZKIEWICZ W., ROMISZOWSKI P., Vacuum **63/64** (2001), 613.

[13] ISO 468, *Surface Roughness – Parameters, Their Values and General Rules for Specifying Requirements, 1982.*

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