Modelling of ceramic coatings grow during Arc-PVD deposition

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Abstract. This paper presents the results of modeling the growth of ceramic coatings obtained by the LDPE method. In the considered model, the possibility of forming misoriented grains relative to each other both in the direction of coating growth and in the growth plane is realized. To verify the model, three coatings of different compositions were prepared and their structure was studied by XRD, TEM, and XPS methods.

1. Introduction

Nowadays, various approaches are used to improve the operational properties of coatings: cerametallic TN-Me, (where T is a transition metal and Me is a plastic matrix of a metal that does not form nitrides), high-hardness coatings (TiN, TiCrN), hardened by ion bombardment, diamond-like coatings (nc-TiN / a-Si3N4), super stoichiometric coating systems TiC_{1+x} or TiC / aC [1–4]. In general, there is a tendency to obtain composite coating materials, where each element has a specific role to play. For example, in CrMoN coatings, chromium provides high oxidation resistance, and molybdenum leads to a decrease in the friction coefficient [5, 6]. The introduction of the copper or nickel into this system leads to an increase in hardness due to the grinding of nitride grains by the metal phase, as well as to an increase in the resistance to viscous fracture due to the same metal matrix [3,7]. This coating technologies are developed is primarily since single-phase systems can no longer satisfy modern requirements. For instance, titanium nitride is characterized by low heat resistance, which levels its high hardness, and as a result limits its use [8]. As a result, scientists have to work with systems consisting of three or more chemical elements. This leads to the difficulty of studying such coatings, since a decrease in the concentration of one component occurs due to an increase in the concentration of other elements. As a result, both the growth regimes thermodynamic parameters of the system can change. In other words, the behavior of such coating systems, depending on the ratio of element concentrations, as well as other application conditions, becomes unpredictable.

In this paper, we propose a model based on the kinetic Monte Carlo method, which, based on data on the concentration flux and phase equilibrium of the system, models the process of coating growth at the atomic level. The use of a stochastic approach reduces the requirements for computing power. In addition, unlike the methods of molecular dynamics, in this model it is much easier to link the evolution of the system to real time [9, 10].

2. Method description

Most computer models of growth of both coatings and other systems are based on the representation of space in the form of cells (Figure 1), which allows us to solve complex geometric problems of crystal

formation, however, such approaches are characterized by a significant drawback - the lack of disorientation of crystals relative to each other, binding of all sizes crystal to cell size, as well as the ability to simulate the phases of only one syngony [11,12]. Figure 1 at the bottom shows an advanced approach that does not fix the center of the atom strictly in the center of the cell, but it can be displaced [13]. It turns out that the cells no longer reflect the space itself but serve only as a tool to accelerate computer calculations. However, even with this approach, the system is characterized by rigid positioning of crystallographic directions in one of the planes. Therefore, if this approach is applied in three dimensions, these models remain pseudo-three-dimensional.

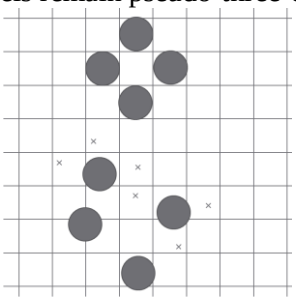

Figure 1. Schematic representation of cell space.

Figure 2 presents a new approach to representing space. As can be seen from the figure, there are no more cells (although they are used in the computer model similarly to the previous approach), the possible positions of neighboring atoms with this approach are determined depending on the group of atoms. If the atom is single, then the possible position of its neighbors is determined by a sphere whose radius depends on the atomic number of the neighbor. The diffusing atom occupies a position characterized by the shortest distance to the atom. As a result, a dimmer is formed - two connected atoms, the axis between which describes the crystallographic direction. Subsequently, upon diffusion of the third atom to the dimmer, it also occupies a position to the nearest accessible position. However, unlike a single atom, in a dimmer, the possible positions are described not by a sphere, but by circles whose radius is determined based on the position of atoms in the lattice sites. And after the addition of the third atom, a full-fledged crystal is formed, for which the possible position of the sites is obtained already by translating the atoms of the crystal lattice.

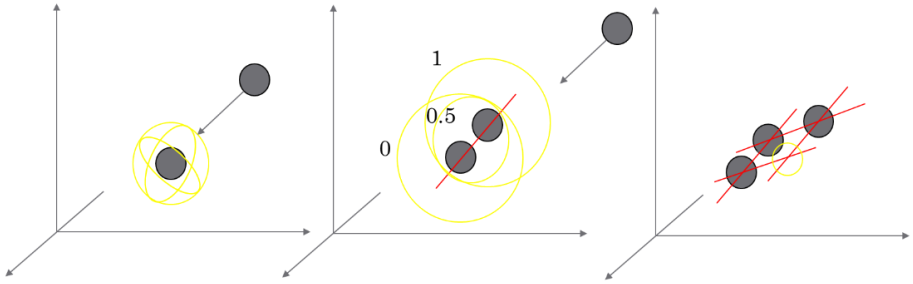

Figure 2. An example of a geometric representation of the formation of dimmers and crystallites.

In this work, we studied the multicomponent Ti-Cr-N-Ni system, which is characterized by the formation of solid solutions of TiN and CrN nitrides with unlimited solubility in each other, and a metal matrix of nickel. To verify the model, three series of coatings were prepared at pAr 0.8 Pa, pN_2 0.4 Pa, a bias potential of 120 V, a substrate temperature of 450 ° C, and the composition shown in Table 1.

Table 1. Elemental composition of coatings obtained by X-ray microanalysis

Concentration, at. %			
Ti	Cr	Ni	N
22	9	14	55
13	36	11	40
10	51	9	30

According to the TEM data, the image of which is shown in Figure 3, all coatings are characterized by a multilayer structure formed as a result of planetary rotation of the substrates.

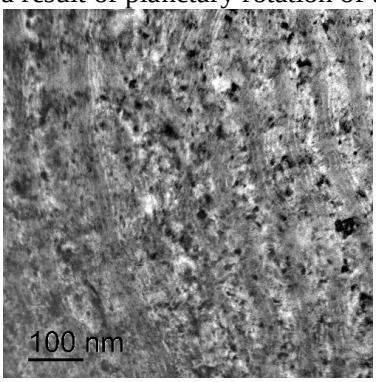

Figure 3. TEM image of the cross section of the coating.

3. Conclusion

The simulation was carried out for systems of 100x100x100 atoms, which made it possible to simulate regions with a size of about 50 nm in height and width, which also corresponds to the modulation period of the coatings obtained. According to the calculations, the layer consists of alternating sublayers with a thickness of 5-6 atomic layers. The formation of such a layer occurs due to the alternating deposition of the products of combustion of the vacuum arc from cathodes of different compositions during rotation of the substrates around its axis. Titanium and chromium are mainly in the nitride phase with a grain size of 3 to 20 nm, while nickel forms crystallites with a size of less than 5 nm as the concentration increases. The proposed model allows us to predict the structure of multicomponent coatings, and as a result, structurally sensitive properties (hardness, wear resistance, optical properties), which can significantly reduce the time and materials spent on scientific research, which at the moment remains purely experimental.

4. Acknowledgments

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5. References

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