



Influence of substrate rotation and target arrangement on the periodicity and uniformity of layered coatings

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ABSTRACT

In physical vapor deposition, the material is vaporized from a target and deposited on the areas of substrate that are in the line-of-sight of a vaporization source. To ensure uniform deposition, substrates are positioned on a turntable and rotated in a manner similar to the planetary rotation. In industrial deposition systems the turntable rotates around several axes and moves substrates along different targets. The substrate rotation and the target arrangement therefore determine the uniformity of the deposited material. When different target materials are used coatings can be prepared in a layered structure; in such a case, the rotation and the target arrangement also determine the layer structure of the coatings. In the present paper a computer simulation of coating growth in an industrial deposition system with a planetary type of rotation has been used to analyze the influence of the rotation and the target arrangement on the uniformity and the periodicity of layered coatings. Results of simulations show that highly periodic modes of rotation, which are determined by the turntable gear ratio and the switch angle, cause large non-uniformities both in the thickness and the composition of layered coatings. On the other hand, less periodic modes of rotation produce better coating uniformity although for certain rotation parameters significant non-uniformities may also occur. Exact periodicity of layered coatings can be calculated from the least common multiple of revolution times around individual axes. Calculations of coating thickness and composition on the perimeter of a round tool show that the uniformity also depends on the deposition time. Configuration with maximally separated targets produces better coating uniformity than configuration with closely positioned targets.

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1. Introduction

Physical vapor deposition (PVD) techniques are widely used methods for the deposition of thin films. In the PVD, the material is vaporized from a target and deposited around the vacuum chamber. In contrast to chemical vapor deposition, the vapor flux in PVD is highly directional since the material originates from a spatially located area, i.e., from a target or more specifically from a small part of the target (e.g. racetrack or cathode spot). Due to directionality of the flux the material is deposited on those surfaces that are in the line-of-sight of the target. Line-of-sight deposition is disadvantageous for many applications where a whole or most of the substrate with complex shape has to be covered.

Several approaches are used to improve uniformity of the line-of-sight deposition. One way is to increase scattering of the vaporized material and thus reduce the directionality of the flux. This can be achieved by working at high pressures where mean free path of the vaporized species is significantly smaller than the target–substrate

distance. Majority of PVD techniques operate at pressures where the mean free path of vaporized species is larger or comparable to the target–substrate distance therefore only a small amount of material reaches shaded areas of a substrate through scattering. High-pressure PVD techniques have been developed to improve uniformity of deposition but such methods are rarely used in practice and acceptable uniformity can be realized only for specific deposition parameters and substrate geometries [1,2]. More importantly, high-pressure PVD techniques are disadvantageous compared to low-pressure PVD techniques since the scattering reduces energy of the vaporized species and thus produces thin films with lower quality.

Uniformity of the deposited material can be also improved if vaporized material is highly ionized and bias voltage is applied to the substrate. PVD techniques with high ionization degree include high power impulse magnetron sputtering and cathodic arc [3]. In the highly ionized plasma, ions are influenced by electric and magnetic fields, thus, they can be guided to those areas that are not in the direct view of the vaporization source. Yet, high ionization degree and biasing do not fully solve the problem of uniformity on large substrates. Ions are guided by electric fields that are mainly present close to cathode [4], biased surfaces and chamber walls (magnetic fields, in e.g. magnetron, are normally too weak to have significant influence on the path of

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ions). Biased or unbiased surfaces immersed in plasma modify plasma potential only in the close vicinity of the surface; the drop in the potential occurs in the so called (pre)sheath area – typically few hundreds of micrometers to several millimeters large [5]. The effect of biasing on the trajectory of ion is thus only felt when ion arrives in the close proximity of the substrate. The advantage of highly ionized plasma on the coating uniformity is evident when coating small features that are in the line-of-sight of vaporization source, such as, trenches with high aspect ratio [6,7]. In cases where large surface areas have to be coated and only part of the surface is in the view of the target (e.g. tools), biasing and the high degree of ionization alone will not enable satisfactory uniformity of the deposition.

The surface of a large substrate can be uniformly coated if several targets are positioned around the substrate. This approach is not practical since it requires several target sources and is only useful for coating one substrate; coating several substrates would be less uniform due to shading by other substrates. The only practical way to improve the uniformity of the deposition in the line-of-sight processes is to rotate the substrates. Rotation ensures that substrates, which usually have complex geometry, are more or less uniformly exposed to the vaporized material. Practically all PVD systems employ some type of substrate rotation which is performed by a turntable. Typically turntables perform planetary type of rotation where turntable rotates around its central axis, while the substrate holders and substrates rotate around their axes.

Industrial PVD systems can be classified into the designs where substrates are always in the view of the vaporization sources and designs where they are not. In the first type of the design the target sources are normally positioned on the bottom of the deposition chamber whereas the turntable is on the top of the chamber. In this configuration, substrates are always in the view of the targets but only one side of the substrate is coated. If the opposite side has to be covered then substrates are turned around and deposition is repeated. PVD systems with the top-bottom design are mainly utilized for the deposition of optical coatings (e.g. anti-reflective coatings on lenses) [8]. The second type of PVD systems employs a design where several vaporization sources (normally four) are positioned around the vacuum chamber in vertical position while the turntable is in the center of the chamber [9,10]. Such design is used for coating the whole surface area of numerous substrates in a single deposition process. The rotation ensures that the surface gets uniformly exposed by all target sources; in this way, a relatively good coating uniformity can be achieved. This type of PVD systems is mainly utilized for the deposition of protective coatings on substrates with complex geometry where small variations in coating uniformity can be tolerated (e.g. tools, machine components, consumer products, medical instruments). In this paper, the analysis of the deposition uniformity will address only this type of deposition systems.

If the rotation in the PVD system is not designed properly, it may cause substantial non-uniformities. In the top-bottom design where substrates are always in the view of the vaporization sources, variations in the deposition rate are minor. On the contrary, in the deposition systems where the turntable is positioned between the vaporization sources, variations in the deposition rate are large. In these systems the distance and the angle between the substrate and individual source change significantly due to rotation. When the substrate travels toward a particular vaporization source, the deposition rate increases to the maximum and decreases when the substrate moves away from the source [11]. If the rotation is highly periodic and substrates return into the same position and orientation for every rotational cycle of the turntable then a large coating non-uniformity will be produced.

The deposition rate variations are especially critical in the reactive deposition mode because they can affect the composition of coatings and, consequently, their properties. In the reactive deposition process the partial pressure of the reactive gas is constant, while the flux of

the material on the surface of the substrate changes due to rotation. Since the ratio between the flux of the reactive gas and the vaporized material is not constant, variations in the stoichiometry can occur. Studies of nanolayered TiAlN/CrN coatings deposited in an industrial magnetron sputtering system with planetary type of rotation revealed that the rotation can produce large differences in the stoichiometry; in some cases, variations were so large that the growth of hexagonal Cr₂N phase was initiated within the cubic CrN phase [12]. It was also shown that variations in the deposition flux caused by the rotation have a strong influence on the microstructure and mechanical properties of coatings [13].

In the literature, the influence of the substrate rotation on the deposition and properties of coatings has not been given much attention; there are only a few studies on this topic [14–18]. Findings in Refs. [12,13] suggest that the rotation should be regarded as one of the deposition parameters since it can significantly influence properties of coatings. Substrate rotation can have an important effect particularly in the case of nanolayered coatings where the thickness of individual layers determines the mechanical properties of coatings. As numerous studies have shown, a very high hardness is obtained only when the thickness of the individual layers is approximately 2–10 nm [19–22]. Substrate rotation can cause significant variations in the thickness of individual layers therefore required layer thickness cannot be satisfied for all layers. The uniformity and the layer structure of nanolayered coatings are also influenced by the target arrangement. Targets can be arranged in different configurations, e.g., targets of the same type can be next or opposite to each other. In nanolayered coatings the sharpness of interfaces plays an important role on the mechanical properties [23] therefore targets should be arranged in such a way that the intermixing between the materials is minimized.

In the present paper, a previously developed computer simulation of coating growth in an industrial deposition system with planetary type of substrate rotation has been utilized [11]. The computer simulation enables calculation of the deposition rate on the surface of a rotating substrate and calculation of individual layer thicknesses that can be visually represented in the form of a layer structure. The accuracy of the calculations was verified by comparing calculated layered structures with the deposited nanolayered coatings [24]. The aim of the present study is to perform computer simulation for different sets of parameters and give a detailed analysis of the substrate rotation and target arrangement on the periodicity and uniformity of layered coatings.

2. Calculation procedure

2.1. Geometry of the deposition system and simulation parameters

Simulations were performed for the magnetron sputtering system CemeCon CC800/9 SinOx ML. A schematic diagram of the deposition systems is shown in Fig. 1. The system has four unbalanced planar magnetron sources with the turntable situated in the center of the deposition chamber. The turntable has six substrate towers and ability of 3-fold planetary type of rotation. Geometry of the CC800/9 system is summarized in Table 1. Rotation around the third axis is non-continuous and is realized by a switch (a metal strip). The switch turns the substrate holder for an angle α for every rotation of the tower around its axis. The revolution time of the turntable can be adjustable from 38 to 97 s, while the revolution time of the substrate tower is determined by the gear ratio (g) between the turntable and the substrate tower. The gear ratio for the CC800/9 system is 100:37 – the turntable gear has 100 teeth while the substrate tower gear has 37 teeth.

Calculations of a layer structure are based on previously developed model of coating growth [11]. The model considers the geometry of the deposition system, rotation of substrates and particle flux from

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