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Influence of the Surface Diffusion Length on the Roughness of Thin Layers Obtained by Random Deposition

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This work identifies a theorical model using the MATLAB software that represents the effect of the surface diffusion length D on the topography and growth dynamics of thin layers obtained by random deposition. The obtained results show that the interface roughness becomes smoother at higher diffusion lengths D. For $D > 0$, the growth exponent β varies according to two distinct regimes, $\beta_1 = 0.5$ presents a completely random growth regime and a constant β_2 presents a diffusion regime of particles towards the hollows, which decreases with increasing D. The interface roughness will never saturate at zero diffusion length, while the roughness exponent takes a lower value of about $\alpha = 0.1450$ at $D = 4$. Finally, the scaling exponents β, α and z directly depend on the diffusion length D and are not related to the substrate size L. The obtained results agree well with other previous theoretical and experimental works.

Keywords: Growth surface, Roughness, Diffusion length, Correlation, Scaling exponents.

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1. INTRODUCTION

The modeling of the coating deposition process by physical or chemical vapor deposition (PVD, CVD) is very complicate and many-sided challenge, which requires versatility [1, 2]. Thus, in the physical deposition film process, film growth depends not only on the interaction of sputtered atoms and the substrate surface, but also on the surface roughness [3]. The formation of defects during the film growth depends on the substrate topography, which is related to preparation steps before the coating process, e.g., polishing and ion etching. Therefore, the surface roughness of the substrate has a significant influence on the adhesion, friction, wear, optical and mechanical properties. A smooth coating surface contact may also increase the adhesion between the surfaces, and therefore, the material transfer between two counterparts will be more pronounced [4].

However, a certain degree of roughness can also be useful for rough sliding surfaces that can store lubricant and supply it to the interface and reduce the abrasive wear. Furthermore, in the sliding test, rougher coating surfaces cause higher friction and low wear resistance because of abrasive and ploughing effects due to smaller real contact area, which increases the tendency for initiation crack and the risk of fatigue-related damage. Thus, the challenge is to find the optimal surface roughness for the contacting surfaces to achieve optimal tribological performance of the coating.

For this reason, much research is aimed at studying the relationship between the surface state, topography of the thin layers growth during continuous bombardment of the interface with atoms using Molecular Dynamics (MD) simulations and Monte Carlo (MC) techniques [5-8]. A big challenge is to understand the interface growth mechanism and the interaction of deposited atoms to predict the topography, thermal and internal stresses of the deposited coating and subsequently to meet the technological requirements [9].

Modeling the non-equilibrium kinetics of crystal growth helps to describe the evolution of the surface as a function of time, since a mentioned interface and a complex structure show common properties such as auto-correlation and self-affinity or self-similarity that facilitates the study of the interface roughness kinetics by scale invariance [10]. The random deposition (RD) model is the best-known basic model that exhibits a discrete network mimicked by sedimentation of particles, where the particle is dropped without predetermining the random site and irreversibly attached [11]. Thus, many statistical models have been developed based on the RD model, including random deposition with diffusion (RDD), where the interface growth is carried out according to the heights of neighboring sites, by appearing height-height correlations [12-15].

Growing surfaces are fractal and evolve naturally to a stable state without a characteristic time scale or length. The development of scaling theory motivated to describe the stochastic dynamics of fractal surfaces as a function of the time of height standard deviation [16]:

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$$W(L,t)=\sqrt{\frac{1}{L}\sum_{i=1}^{L}\left[h(i,t)-\bar{h}(t)\right]^{2}}\,, \qquad (1)$$

where W is the surface roughness, L is the system size, $h(i, t)$ is the height of the site surface i in time t, and $\bar{h}(t)$ is the average height of the surface at time t, which is calculated by the following equation:

$$\bar{h}(t)=\frac{1}{L}\sum_{i=1}^{L}h(i,t)\,. \qquad (2)$$

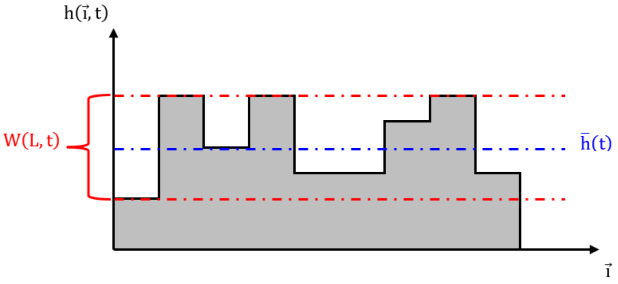

Fig. 1 – Schematic presentation of the surface cross-section at time t, showing the surface roughness $W(L, t)$ and the average height of the surface $\bar{h}(t)$

The majority of growth models are based on the global interface roughness scaling relation (also called the family-Vicsek scaling relation):

$$W^{2}(L,t)=L^{2\alpha}f\left(\frac{t}{L^{z}}\right)\sim\begin{cases}t^{2\beta} & \text{for } t\ll L^{z}\\ L^{2\alpha} & \text{for } t\gg L^{z}\end{cases} \qquad (3)$$

This relation implies that the width of the interface roughness increases as the power of time increases $W(t)\sim t^{\beta}$ from t_x, $t\ll t_x$, called time of saturation [17], where β is the growth exponent that describes the time-dependent surface roughness dynamics, α is the roughness exponent that describes the roughness after system saturation. There is a strong relationship between the two exponents when describing the dynamic scaling exponent $z = \alpha/\beta$ [18].

To study the height-height surface correlation, it is important to involve the space-time correlation function (C) by defining the difference in height between two interface positions that are separated by the distance x at the deposition time t [19].

$$C(x,t)=\left(h(x_0+x,t)-h(x_0,t)\right)^{2}_{x_0}\,. \qquad (4)$$

2. MECHANISM OF SURFACE GROWTH BY DIFFUSION

Surface growth in this model is based on RD by adding a limited length of surface diffusion (D), which causes a superficial relaxation, and its effects are similar to surface tension in the liquid surface. The growth occurs on a substrate of length $L = P/10$ (P is the number of particles bombarding the substrate), where the particles, instead of immediately sticking to the cluster at site i of height h_i, diffuse and stabilize at more stable sites located at a given distance ranged between $(i - D)$ and $(i + D)$ (the particles roll in hollows). The restructuring is dominant, where the state of the obtained interface is now sensitive to the diffusion length D. The growth conditions are summarized as follows:

- The substrate contains a number of sites $i\in[1,\dots,L]$, where the periodicity between the ends is preserved $(L+1\equiv 0 \text{ et } 0\equiv L)$.
- If $h_i>\min\{h_j, j\in[i-D,i+D]\}$, the particle will seek to stick in one of the neighboring sites, from $[i-D,i+D]$ a minimum height with 80 % probability, or 20 % to stay where it fell.
- If $h_i<\min\{h_j, j\in[i-D,i+D]\}$, the particle sticks irreversibly in site i with a probability of 100 %.
- If $h_i=\min\{h_j, j\in[i-D,i+D]\}$, the particle crashes into one of the sites $i-D$ or $i+D$ with equal probability.

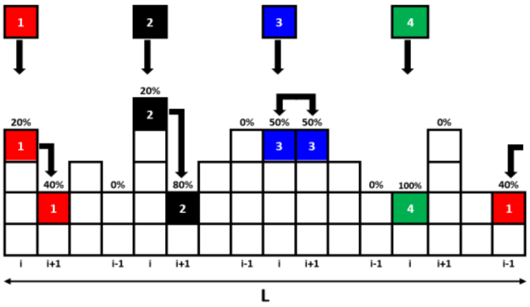

Fig.2 – Illustration of the growth mechanism in the random deposition with a diffusion length $D = 1$

3. RESULTS AND DISCUSSION

3.1 Topography and Scaling Behavior

Fig. 3 presents the surface topography of thin layers obtained by random deposition with different diffusion length ($D = 0$, 1, 2 and 4). For $D = 0$, the interface is completely rough, and the interface roughness varies between 5 and 15, because particles were deposited in a random way and stuck irreversibly in the random site i. When $D = 1$, the interface roughness slightly improves, and the layer surface becomes smooth due to the diffusion of particles towards neighboring sites of a minimal height ($i - 1$, $i + 1$). The surface becomes smoother, and the roughness (surface height) reaches a lower value of about 2 at $D = 4$, when the particles move to fill the lower troughs of the farthest neighboring sites ($i - 1$, $i - 2$, $i - 3$, $i - 4$ and $i + 1$, $i + 2$, $i + 3$, $i + 4$).

In hard thin films, the roughness has an important effect on the mechanical, wear and corrosion resistance. Zhang et al. [20] found that a rougher surface can affect the resulting hardness and elastic modulus during nano-indentation. Other hind, J. Munemasa et al. [21] reported that sputtered TiN films with a smoother substrate surface have high hardness and better corrosion resistance. In our case, a smooth surface with a lower roughness of films deposited at D ranged between 2 and 4 can be used to obtain functional properties.

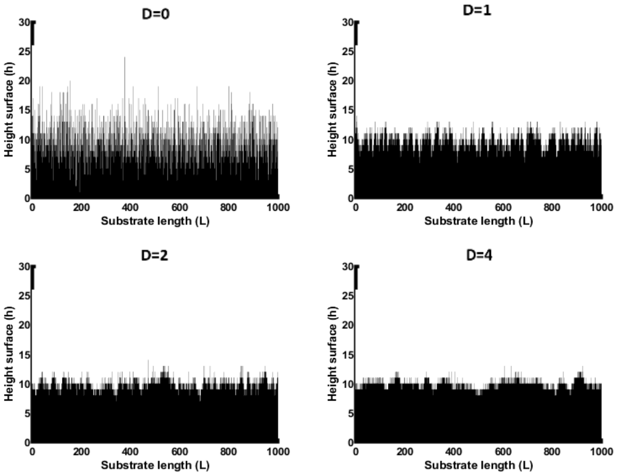

Fig. 3 – Surface topography of thin layers obtained by random deposition with different diffusion lengths D) keeping constant the substrate size $L = 1000$ and the number of bombarding particles $P = 10000$

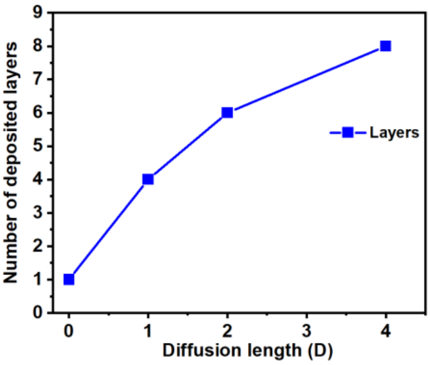

Fig. 4 – Surface evolution of the number of deposited thin layers as a function of diffusion length D

Furthermore, the diffusion length D is directly affected by the number of layers deposited during film growth. For $D = 0$, the formed surface contains four thin layers. For this type of structure, we can observe high surface roughness with more defects that are generated at the film surface.

The number of thin deposited layers increased with increasing diffusion length D and reached the number of thin layers of about eight at $D = 4$ (Fig. 4). With increasing the number of layers, the structure becomes denser, soother and more homogeneous due to the high mobility of atoms during the deposition process and the low surface energy of this film, which leads to a rounded grain shape [22]. This type of structure can be useful for increasing the fatigue wear resistance of coatings [23].

To study the growth mechanism of thin layers obtained by random deposition with surface diffusion and its effect on roughness, Fig. 5 shows curves of interface roughness (W) as a function of time (t) for different substrate sizes (L) and diffusion lengths (D). It is observed that the layers obtained by RDD were constructed in two distinct regimes. Initially, the growth is completely random since the particle diffusion process does not matter because the number of particles deposited is less than the size of the substrate L. After the creation of the first layers, the diffusion of particles limits the growth of the interface, persisting more and more with larger D where the growth regime has a tendency towards saturation as a function of time t. However, the growth regime is not affected by the substrate size L, and only the size of the system has increased (Fig. 5a).

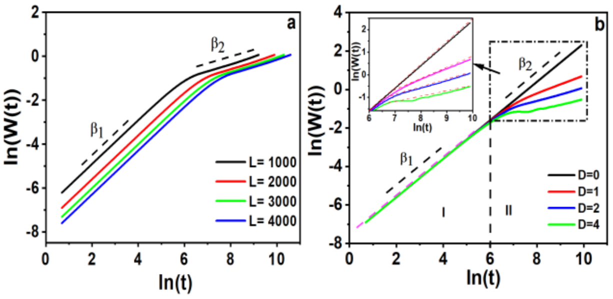

Fig. 5 – Growth of rough surfaces (W) as a function of time (t): (a) for different sizes of the substrate L and the number of bombarding particles P where $D = 2$ is kept constant; (b) for different diffusion lengths D, where $L = 1000$ and $P = 10000$ are kept constant (the averages are calculated at Test = 1000 different configurations)

The surface growth regime is characterized by the exponents β_1 and β_2 which are calculated from the slope of the interface roughness growth (W) as a function of time (t). For $D = 0$, we can notice $\beta_1 = \beta_2 = 0.5$, which is a completely random growth with an autonomous regime never reaching saturation. The situation changes radically for $D > 0$, where $\beta_1 \neq \beta_2$, which vary according to two distinct regimes. At the fist start of deposition, the interface roughness grows rapidly, following a transient linear regime with growth exponent $\beta_1 = 0.4975$, corspending to the random deposition regime. Then, the growth regime has a tendency towards saturation by decreasing the growth exponent down $\beta_2 = 0.2954$ for a larger diffusion length $D = 4$. Similar observations were found by M. Claudio et al. [24].

Table 1 – Average values of the growth exponents β_1 and β_2 for different diffusion lengths (D), where $L = 1000$ and $P = 10000$ are kept constant

D	β_1	β_2
0	0.5	0.5
1	0.4975	0.4595
2	0.4991	0.3617
4	0.4985	0.2954

Table 2 – Average values of the roughness exponent α and the dynamic exponents z_1 and z_2 for different diffusion lengths (D), where $L = 1000$ and $P = 10000$ are kept constant (the averages are calculated at Test = 1000 different configurations)

D	α	z_1	z_2
0	0	0	0
1	0.5519	1.1093	1.2010
2	0.3361	0.6734	0.9292
4	0.1450	0.2908	0.4908

The roughness exponent α describes the interface roughness after saturation of the system, which was calculated by the slope of the correlation region C and the height difference between two interface positions separated by a distance x (Fig. 6). It can be seen that

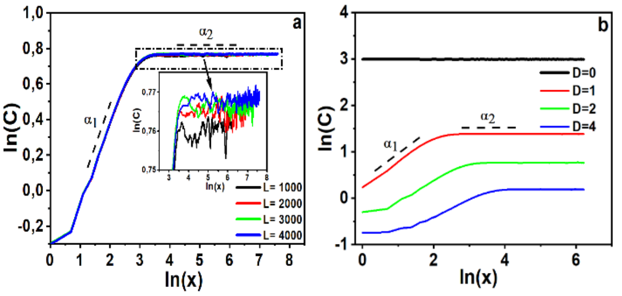

Fig. 6 – Roughness height correlation *C* between two interface positions separated by distance *x* generated by the deposition (RDD): (a) for different sizes of the substrate *L* and the number of bombarding particles *P* where $D = 2$ is kept constant; (b) for different diffusion lengths *D*, where $L = 1000$ and $P = 10000$ are kept constant (the averages are calculated at Test = 1000 different configurations)

the surface correlation depends on the diffusion length *D* and that an increase in the substrate size *L* has no influence on the interface state. At the same time, when the length is zero, it was found that each update does not correlate with the previous one and that the spatial correlation function $C(x)$ remains flat with a roughness exponent $\alpha = 0$ due to the effect of the lack of organization of a regular interface and the absence of interactions between heights of neighboring sites. On the contrary, the interface roughness becomes smoother with a larger scattering length. But the interface roughness remains rough on large scales, where the roughness exponent α decreases with increasing scattering length.

4. CONCLUSIONS

In this work, we used Monte Carlo simulations to study thin layers obtained by the random deposition (RD) as a function the surface diffusion length *D*. The conclusions are summarized as follows.

- Thin layers obtained by the random deposition with diffusion (RDD) have a smooth surface with less roughness than that obtained by random deposition (RD).

- The diffusion length *D* is not affected by the growth regime of the first layers, while it is effective afterwards.

- The scaling exponents β, α and z are proportional to the scattering length *D*, however, they are independent of the substrate size *L* and the number of bombarding particles *P*.

- All thin layers obtained in the RDD mode are correlated, in contrast to the RD mode.

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Вплив довжини поверхневої дифузії на шорсткість тонких шарів, отриманих випадковим осадженням

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У роботі описано теоретичну модель з використанням програмного забезпечення MATLAB, яка описує вплив довжини поверхневої дифузії D на топографію та динаміку росту тонких шарів, отриманих шляхом випадкового осадження. Одержані результати показують, що поверхня інтерфейсу стає більш гладкою при більшій довжині дифузії D. Для $D > 0$ показник росту β змінюється відповідно до двох різних режимів, $\beta_1 = 0{,}5$ представляє повністю випадковий режим росту, а показник β_2 представляє режим дифузії частинок у напрямку до пустот, β_2 зменшується зі збільшенням D. Шорсткість інтерфейсу ніколи не насичується при нульовій довжині дифузії, тоді як показник шорсткості приймає нижче значення приблизно $\alpha = 0{,}1450$ при $D = 4$. Нарешті, коефіцієнти масштабування β, α та z безпосередньо залежать від довжини дифузії D і не пов'язані з розміром підкладки L. Отримані результати узгоджуються з іншими попередніми теоретичними та експериментальними роботами.

Ключові слова: Поверхня росту, Шорсткість, Довжина дифузії, Кореляція, Коефіцієнти масштабування.