



The pressure dependence of the deposition rate in a magnetron sputtering system



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ARTICLE INFO

Article history:

Received 3 April 2014

Received in revised form 11 November 2014

Accepted 12 November 2014

Available online 20 November 2014

Keywords:

Magnetron sputtering
Pressure–distance product
Thermalization length
Multicomponent film

ABSTRACT

An analytical expression is obtained for the pressure distance product parameter that defines the pressure dependence of the deposition rate of sputtered atoms in the Keller–Simmons formula. The generalized Keller–Simmons formula is proposed, which can be used in the case when the 1D approach is not suitable for the simulation of the flux of sputtered atoms to a substrate. The generalized Keller–Simmons formula using the pressure distance product derived from the analytical expression allows one to simulate the pressure dependence of the deposition rate of sputtered atoms for different target materials and to simulate the chemical composition of a multicomponent film at different pressures and distances from a compound target to the substrate. Results of simulations using the generalized Keller–Simmons formula are in good agreement with the experiment.

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1. Introduction

Magnetron sputtering systems are widely used for thin film deposition [1–3]. Characteristics of films depend on many parameters of the deposition process, especially the energy of sputtered atoms that reach the substrate [1] and the angular distribution of sputtered atoms on the substrate [4,5]. In the case of a multicomponent target used for the deposition of a multicomponent film, the film's characteristics significantly depend on the chemical composition of the film [6,7]. Changing the pressure or a target–substrate distance results in a change of the number of collisions of sputtered atoms with gas atoms. The collisions change the energy and path of the sputtered atoms and thus change the energy, the angle of incidence and the deposition of sputtered atoms on the substrate. The change of the deposition rate due to collisions will be different for sputtered atoms with different masses. This is why the content of different components in the film can be controlled by changing the pressure or the target–substrate distance.

Exact modeling of the transport of sputtered atoms in a magnetron discharge should include accurate modeling of the energy and angular distributions of atoms sputtered from the target. These distributions depend on a target and on the energy of plasma ions bombarding the target [8]. Experimental data of the energy and angular distributions of sputtered atoms do not always exist. Sometimes, in Monte Carlo simulations, these distributions are estimated using specialized software such as the freeware software SRIM or TRIM, see, e.g., [9]. More frequently, the energy and angular distributions of sputtered

atoms in Monte Carlo simulations are defined by simple functions. The energy distribution function of the sputtered atoms is frequently defined by the Thompson energy distribution [10] or some of its modifications [11–13]. The angular distribution function of the sputtered atoms is defined either by a cosine distribution [11] or a \cos^n distribution [12]. According to [11–13], such approaches provide a good correlation between simulations and the experiment. Although these simplified approaches can be used in the modeling, the Monte Carlo simulation is, as a rule, time consuming.

To have an algorithm for fast estimation of the pressure effect on the deposition rate, we need a physically approved analytical expression for the simulation of the deposition rate of sputtered atoms. Magnetron sputtering systems are characterized by small enough pressures so that fluxes of both thermalized and fast non-thermalized sputtered atoms to the substrate should be taken into account in the simulation of the deposition rate. Such an analytical expression was initially proposed by Keller and Simmons [14] in the following form:

$$\Phi = \Phi_0 \frac{3\lambda}{2d} \left(1 - \exp\left(-\frac{2d}{3\lambda}\right) \right)$$

where Φ_0 is the flux of atoms sputtered from a target, Φ is the flux of atoms deposited on a substrate, d is the target–substrate distance and λ is the mean free path of sputtered atoms in a discharge. The pressure dependence in the equation is governed by the mean free path that is inversely proportional to the discharge gas concentration. It should be noted that the Keller–Simmons formula was obtained in [14] using a 1D approach, which implies that the target diameter is significantly larger than the target–substrate distance. The Keller–Simmons formula

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can be written in another form, see, e.g., [15]:

$$\Phi = \Phi_0 \frac{(pd)_0}{pd} \left(1 - \exp\left(-\frac{pd}{(pd)_0}\right) \right) \quad (1)$$

where p is the pressure in a deposition chamber and $(pd)_0$ is the characteristic pressure–distance product. In many publications [15–22], it is shown that experimental pressure dependencies of the deposition rate are well reproduced by the Keller–Simmons formula (Eq. (1)). However, the parameter $(pd)_0$ introduced in Eq. (1) is initially unknown and is usually considered as a fitting parameter. In [15–17], it is shown that the parameter $(pd)_0$ of Eq. (1) depends on the target material, type of gas and sputtering power. According to Palermo [22], the $(pd)_0$ parameter can be treated in the form:

$$(pd)_0 = p\Lambda \quad (2)$$

where Λ is the thermalization distance for sputtered atoms.

The dependence of $(pd)_0$ on sputtering power according to [16,22] is caused by the rarefaction effect resulting from the heating of the gas in the process of the thermalization of sputtered atoms. In the case of high power deposition, the increase of the gas temperature can be significant [12,16]. The accurate modeling of the transport of sputtered atoms under such conditions should be self-consistent, including modeling of the rarefaction effect [12]. Experiments performed with different target materials [16] show that at small magnetron powers the gas heating caused by the degradation of energy of sputtered atoms is not significant. Thus, the results of simulating the transport of sputtered atoms using the initial gas temperature will be reliable for the case of low power deposition.

In this paper, we restrict our considerations only to the case of low power deposition. We propose an analytical expression of $(pd)_0$ through the characteristics of sputtered and gas atoms at a given gas temperature. The knowledge of the $(pd)_0$ parameter will allow one to make estimations of the pressure effect on a deposition rate without preliminary experimental investigations. It also gives one an ability to estimate the parameters p and d at which sputtered atoms deposited on the substrate will be mainly non-thermal. In the case of a multicomponent film, the knowledge of $(pd)_0$ parameters for different components gives us the ability to estimate the effect of the pressure and the target–substrate distance on the chemical composition of the film. The generalized Keller–Simmons formula will be proposed in the paper to be used in the case when the 1D approach is not suitable for the simulation of the flux of sputtered atoms to a substrate.

2. Theory

In the beginning of this section, our consideration will be confined to the 1D approach corresponding to Eq. (1). Later on, results will be generalized to more complex geometry configurations where the 1D approach is not accurate. According to Eq. (2), the parameter $(pd)_0$ of the Keller–Simmons formula (Eq. (1)) can be defined through the thermalization length Λ , which is the distance from the target surface to a position where the sputtered atoms become thermal due to the degradation of their energy in collisions with gas atoms. The average number of elastic collisions required for the thermalization of sputtered atoms was estimated in [22] through $(pd)_0$ parameters obtained by fitting the Keller–Simmons formula (Eq. (1)) with experimental dependencies of $\Phi(p)$ from [15–17]. The estimated numbers of elastic collisions for different target materials were compared in [22] with the analytical results of [23]. The comparison showed a good correlation of estimated and analytical results. Let us note that in [23] three different approaches were considered to define the number of collisions required for the thermalization, but in [22] it is not specified which of the approaches was used for the comparative analysis. By comparing Fig. 3 of [22] and Fig. 4 of [23], one can conclude that the number of

collisions defined by Eq. (8) of [23] that take into account the concept of persistence of velocity after collisions [24] was used in the comparisons of [22]. In essence, the results of [22] demonstrate that using the thermalization distance D_3 , introduced by Eq. (11) of [23], as the thermalization length Λ in Eq. (2) allows one to reproduce the trend of the $(pd)_0$ parameter on the mass ratio of sputtered atoms to the gas atoms.

Detailed analysis shows that the analytical results of [23] are obtained using fairly rough approaches and the thermalization distance definition should be corrected. In [25], the transport of sputtered atoms was simulated by the Monte Carlo method in a wide range of variation of energies of sputtered atoms and mass ratios of sputtered atoms to the gas atoms. The thermalization distances h calculated by means of the Monte Carlo simulations were fitted in [25] by the following relation:

$$h = \lambda_0 \cdot (m_1/m_2)^{0.69} [0.39 + 0.23 \ln(E_0/E_{th})] \quad (3)$$

where E_0 is the initial energy of sputtered atoms, E_{th} is the thermal energy of gas atoms given by $E_{th} = 3kT/2$, where k is the Boltzmann constant, T is the gas temperature, m_1 is the mass of the sputtered atom, m_2 is the mass of the gas atom, and $\lambda_0 = 1/(n\sigma)$, where n is the discharge gas concentration and σ is the cross section of elastic scattering of the sputtered atom by the gas atom.

Approaches used in [25] provide more accurate modeling of the sputtered atoms transport compared with the approaches used in [23]. The stochastic nature of the collisions of sputtered atoms with gas atoms is taken into account in [25] in contrast to the approaches of [23], where the energy of a sputtered atom after each elastic collision is simulated through the average energy loss. Unlike the approach of atoms sputtered normal to the target surface used in [23], a cosine-angle distribution of atoms sputtered from the target surface is considered in [25]. A Maxwellian energy distribution of gas atoms is taken into account in [25] in contrast to immobile gas atoms considered in [23]. Let us note that Monte Carlo simulations show that the motion of gas atoms can significantly affect the transport of sputtered atoms [26]. The thermalization length is calculated in [23] using the following mean free path λ of sputtered atoms between subsequent elastic collisions:

$$\lambda = \lambda_0 / \sqrt{1 + m_1/m_2}. \quad (4)$$

We should emphasize that, according to [24,27], Eq. (4) corresponds to the mean free path of atoms that are already thermalized. In the case of fast, non-thermalized atoms, the mean free path of the atoms depends on their velocity [24,27]. The convenient form of such dependence expressed through the energy of atoms E is presented in [25] by the following equation:

$$\lambda = \lambda_0 \left[\left(1 + \frac{1}{2\omega} \right) \operatorname{erf}(\sqrt{\omega}) + \frac{e^{-\omega}}{\sqrt{\pi\omega}} \right]^{-1} \quad (5)$$

where erf is the error function [28], $\omega = \frac{3}{2} \frac{E}{E_{th}} \frac{m_2}{m_1}$. It is seen from Eq. (5) that at high energies of sputtered atoms corresponding to $\omega \gg 1$, the mean free path λ will be close to λ_0 and it will be higher than the one defined by Eq. (4), especially in the case of $m_1 > m_2$. The dependence of the mean free path λ of sputtered atoms from their energy E which changes due to collisions is taken into account in [25]. The cross section of elastic scattering in [25], as well as in [23], was derived through the radii of the sputtered and the gas atoms by the relation $\sigma = \pi(r_1 + r_2)^2$.

The thermalization length h defined by Eq. (3) and the thermalization length D_3 defined by Eq. (11) of [23] are compared in Fig. 1 for two different initial energies of sputtered atoms. It is seen that slopes of the dependencies $h(m_2/m_1)$ and $D_3(m_2/m_1)$ are different. The ratio of masses m_2/m_1 at which the dependencies agree well changes with the change of initial energy of the sputtered atoms. Approaches used in [25] provide a more realistic description of the transport of sputtered

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