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The influence of target surface morphology on the deposition flux during direct-current magnetron sputtering

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1. Introduction

Modeling the growth of thin films is a challenging endeavor that requires a good understanding of several processes and the parameters that drive them. The material flux towards the substrate, and the energy distribution of the arriving atoms plays a key role [1]. For magnetron sputter deposition this translates to the sputter yield and the angular distribution profile. The first determines the amount of atoms that will enter the gas phase and the second describes the direction in which the sputtered atoms are ejected from the target.

The sputter yield of a material is defined as the number of atoms that are sputtered per incoming ion. For an atomically flat surface. this is a well defined quantity. However, when a real target with a specific surface morphology is used, it is recommended to distinguish between the 'elemental sputter yield' and the 'effective sputter yield' of the target. The effective sputter yield in that case is defined as the number of atoms that leave the target per incoming ion. This value can deviate from the elemental sputter yield due to the target surface morphology [2–5]. The effect is twofold and is depicted in Fig. 1, which schematically represents a not atomically flat surface. First of all, due to the fact that a real surface is composed of hills and valleys, the ions will impinge the target surface under an angle θ rather than under normal incidence. This leads to a local increase of the elemental sputter yield [6-8]. Secondly, atoms that are being sputtered from a rough surface have a probability to get redeposited onto the target due to the geometry of the surface, which results in a lower effective

ABSTRACT

The effect of the target surface morphology on the sputter deposition flux and the energy flux is investigated by comparing solid targets to pressed powder targets. A significant, material dependent difference of the effective sputter yield between both target types is noticed. This difference is explained by combining two effects: a local increase of the elemental sputter yield and the redeposition of sputtered atoms onto the target. Both effects strongly depend on the target surface morphology. The experimental trends are reproduced by Monte Carlo simulations. This allows a description of the angular distribution of the sputtered atoms which is an important parameter to define the particle flux and the energy distribution of the atoms arriving on the substrate. Using the previously developed particle trajectory code SIMTRA, the latter is demonstrated for the studied materials (Al, Ag, Cu, and Ti).

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sputter yield. Hence, the global change in the effective sputter yield will be determined by the dominating effect.

It should be noted that not only redeposition will have an influence on the effective sputter yield. When ions approach the target under an oblique angle relative to the target normal, part of the surface may be shadowed from the ions. This might be the case during ion beam sputtering with a non-zero nominal angle of incidence [2]. However, during magnetron sputtering the nominal angle of the incident ions is always zero. This is based on the assumption that the macroscopic dimensions of the cathode sheath are not influenced by the microscopic morphology of the target. Hence the ions are always accelerated parallel to the target normal. Therefore this shadowing effect is not taken into account here.

The angular distribution of atoms ejected from a target which is bombarded by energetic ions under normal incidence is generally a cosine-type distribution [6,9]. The orientation of the hills and valleys will however also influence the shape of this profile as the inclined planes will promote the ejection of atoms along the local surface normal, rather than the target normal. This can result in typical heart-shaped or under-cosine profiles which have been observed experimentally [10–13].

In this work the influence of the target morphology is investigated by measuring the effective sputter yield of four different materials (Cu, Al, Ti and Ag), using both solid targets as well as uniaxially pressed powder targets. The observed discrepancy in the sputter yield of each material, depending on the kind of target that is used, can be understood and explained by the observed differences in surface morphology. A combination of SRIM [14] simulations and an in-house developed Monte Carlo (MC) code is used to quantify the deviations of the effective sputter yields. The MC code furthermore allows the construction of the



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Fig. 1. Schematic representation of a rough surface and its influence on the sputter yield. An ion strikes the surface under an angle *θ*. The small dashed line is the local surface normal. Particles that are sputtered below the large dashed line will get redeposited onto the target surface.

global angular distribution of the ejected atoms, which in turn is used as input for the previously developed particle trajectory code SIMTRA [15,16]. These latter simulations show the influence of the angular distribution on the deposition rate and the energy flux towards a substrate during sputter deposition.

2. Experimental details

All experiments were carried out in a stainless steel vacuum chamber. A turbomolecular pump, backed up by a rotary pump was used to pump down the chamber to a base pressure of 10^{-4} Pa. The solid targets were 99.99% pure Cu, Al, Ti and Ag targets from Kurt J. Lesker with a diameter of 50.8 mm and a thickness of 3 mm. The pressed powder targets were obtained by pressing 99% pure Cu. 99.5% pure Al. 99.99% pure Ti and 99.99% pure Ag into a solid disk shape. For mechanical reasons, stainless steel rings were used with an inner and outer diameter of resp. 46 and 50.8 mm and a thickness of 2 mm. A maximum isotropic pressure of 15 tons was applied. The maximum grain size of the powder atoms was 50 µm for the Cu and Al (Goodfellow), 45 µm for the Ag (Goodfellow) and 44 µm for the Ti (Alfa Aesar). These pressed powder targets were then mounted onto a 1 mm thick copper plate with a diameter of 50.8 mm, resulting in a pressed powder target with the same dimensions as the solid targets. All targets were mounted onto an unbalanced magnetron powered by a Huttinger DC power supply and sputtered for several hours in a pure Ar atmosphere of 0.4 Pa at constant discharge voltage. These experiments were repeated for each target material for different discharge voltages. The mass of the targets before and after sputtering was determined by a microbalance with a resolution of 1 mg. From the mass difference, the effective sputter yields were determined (see Section 3.1). In order to check whether material loss occurred due to evaporation or mechanical fall off of the powder, the targets were also weighed before mounting them into the chamber and again after several hours of pumping. No difference in mass was observed, which evidences that evaporation and mechanical fall off can be neglected.

The surface morphology of the targets was measured with an optical profilometer (WYKO NT3300). Before sputtering, each target was scanned over three randomly selected sample areas of 242.1 by 184.2 μ m with a resolution of 328.95 nm in both *X* and *Y* direction. The same measurements were again carried out on each target inside the racetrack after sputtering.

3. Results and discussion

The yield measurements and the target surface analysis are described in Sections 3.1 and 3.2. Section 3.3 describes how the effective sputter yield can be calculated from the elemental sputter yield. It is shown that two parameters are needed in order to do this: the yield amplification factor α and the atom redeposition probability factor $1-P_{\lambda}$. The calculation of these factors is described in Sections 3.3.1 and 3.3.2 respectively. Next, in Section 3.3.3, these two factors are combined to reproduce the measured effective sputter yields. Finally, the angular distributions of sputtered atoms are calculated and used to simulate the deposition flux. These results can be found in the Sections 3.4 and 3.5.

3.1. Sputter yield measurements

The effective sputter yield of all targets was determined from the mass difference Δm before and after several hours of sputtering at a constant discharge voltage. As discussed in [17–19], the effective sputter yield Y_{eff} can be retrieved from this mass difference using the following equation:

$$Y_{eff} = \frac{\Delta m \cdot N_A}{M} \cdot \left(\frac{\sum_t I_t dt}{e \cdot (1 + \gamma_{isee})}\right)^{-1}$$
(1)

where N_A is Avogadro's constant, M is the molar mass (g/mol) of the material, I_t (C/s) is the discharge current at time t, dt is the time interval between two measurements of I_t , e is the elementary charge (C) and γ_{isee} is the ion induced secondary electron emission yield [20,21].

Fig. 2 shows the measured sputter yields of different materials obtained by sputtering from the powder and solid targets as described in Section 2. The difference between the effective sputter yields of the powder targets and those of the solid ones is quite remarkable. Furthermore this appears to be material dependent. While on average there is a decrease of 16% and 24% from solid to powder target for Ag and Cu resp., there is an average increase of48% for Al. No significant change in sputter yield observed for the Ti targets.

3.2. Target surface analysis

The data file of each optical measurement is a matrix containing the measured height of each data point. From this matrix a submatrix of 100 by 100 μ m was selected for further analysis.

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