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Modeling target erosion during reactive sputtering

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ABSTRACT

The influence of the reactive sputter conditions on the racetrack and the sputter profile for an Al/O_2 DC reactive sputter system is studied by modeling. The role of redeposition, i.e. the deposition of sputtered material back on the target, is therefore taken into account. The used model RSD2013 is capable of simulating the effect of redeposition on the target condition in a spatial resolved way. Comparison between including and excluding redeposition in the RSD2013 model shows that the in-depth oxidation profile of the target differs. Modeling shows that it is important to distinguish between the formed racetrack, i.e. the erosion depth profile, and the sputter profile. The latter defines the distribution of the sputtered atoms in the vacuum chamber. As the target condition defines the sputter yield, it does determine the racetrack and the sputter profile of the planar circular target. Both the shape of the racetrack and the sputter profile change as function of the redeposition fraction as well as function of the oxygen flow change. Clear asymmetries and narrowing are observed for the racetrack shape. Similar effects are noticed for the sputter profile but to a different extent. Based on this study, the often heard misconception that the racetrack shape defines the distribution of the sputtered atoms during reactive sputtering is proven to be wrong.

1. Introduction

The study of sputter deposition was initiated in 1852 by Grove [1] while studying a glow discharge. Nowadays it is known that due to the bombardment of the cathode by energetic ions from the plasma, target atoms are ejected into the vacuum and are deposited on a substrate. In present setups there are usually magnets to localize the generated plasma closely above the target surface, which greatly enhance the sputtering [2]. The sputtered atoms have typically starting energies of up to tens of eV [3]. At low gas pressure and/or short target-substrate distance, these sputtered atoms will travel in an almost straight line and energetically impact on the substrate. If the gas pressure is sufficiently high and/or the target–substrate distance is relatively long, then the sputtered atoms will more frequently collide with background gas atoms. In this way their movement becomes diffusive and they thermalize due to energy transfers. When reaching the substrate, they will condense on it at thermal energy [4,5]. Besides this desired deposition of material on the substrate surface, there will also occur deposition on the chamber walls and some deposition back on the target. The latter phenomenon is commonly called redeposition [6]. This redeposited material back on the target is then available to be sputtered, but evidently this phenomenon reduces the efficiency of the sputter process.

In non-reactive sputter deposition, the redeposited material on the target is the same as the initial target material. When moving to reactive sputter deposition where a reactive gas is added to the system, the picture changes. The purpose of the reactive gas is to deposit a compound film on the substrate by chemical reaction of the gas with the deposited target material. However compound formation can also occur on the target itself, where it is subject to sputtering. As such the (re)deposition flux will be a mixture of compound constituents and original target material. In this way the effect of redeposition also defines the level of compound formation on the target. Considering redeposition in reactive sputter systems is then of technological importance as it influences the arcing behavior and the racetrack formation. Segers et al. [7] argued that arcing seriously intensifies when a certain critical compound thickness is reached. The spots of arcing are then located at the racetrack rim where porous, non-stoichiometric compound is formed. The growth of this compound layer is due to redeposition. Also the racetrack formation will be altered due to redeposition. Redeposition will non-uniformly reduce the erosion rate of the target, as it plays a role in the compound formation and as it returns sputtered material.

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In our perspective of modeling [8,9], three pathways of compound formation on the target are considered. Firstly, reactive gas molecules can chemisorbed on non-reacted target material. Secondly, as the reactive gas will also be partially ionized they will also bombard the target and get implanted below the surface. These implanted reactive gas atoms can then chemically react with the target metal. Finally, redeposition of both reactive and non-reactive sputtered material on the target influences the dynamics of compound formation. This compound formation on the target is often the cause of a hysteresis phenomenon in the reactive sputter process [10]. Hysteresis can, for example, be observed when the reactive gas flow is stepwise increased and subsequently decreased, without changing other operation settings. Some of the observables, like the pressure, will then describe a hysteresis loop, meaning that the observable will be double valued at some range of reactive flow values. The actual value will then depend on the history of the system. The emergence of this hysteresis is due to a much lower sputter yield of the compound compared to the original target material. Its behavior as function of the process parameters is already frequently studied as well experimentally as by modeling [11]. However, studies of the influence of the redeposition fraction on the reactive sputter process are limited [9,12]. Here, this influence will be studied by modeling the process and it will be shown how it impacts on the racetrack and the sputter profile.

The first researchers who included the process of redeposition in a reactive sputter model were Depla et al. [9]. With his model RSD2009 he investigated the importance of redeposition for a rotatable cylindrical DC magnetron. Here the redeposition will be considered for a static, planar, circular magnetron with an updated version of the RSD model, namely RSD2013. This model, like RSD2009, basically describes the evolution of the compound formation on target and substrate, and of the reactive gas pressure. The full description of RSD2013 [8] and the software [13] itself was published earlier. The RSD model can especially include the effect of redeposition for evaluating its influence on the hysteresis. The fraction of the sputtered flux which is redeposited and its distribution over the target is an input for the RSD model. This input can be calculated by the Monte Carlo program SIMTRA [14,15]. Combining RSD2013 and SIMTRA with the program SRIM, which simulates ion–solid interactions, enables to model the reactive sputter process.

Section 2 presents some relevant equations and definitions of the RSD2013 model for the target description. Results and discussion of the influence of the redeposition fraction along the hysteresis curve is evaluated in Section 3. Besides this impact on the pressure-flow hysteresis curve, the effect on the racetrack and the sputter profile is also examined as function of the reactive gas flow and of the redeposition fraction. Finally, a conclusion is given in Section 4.

2. The model

As the focus here will be on the target evolution along the hysteresis curve and of the racetrack and sputter profile of the target, this section only summarizes the target description of the RSD2013 model in its time dependent formulation. A full and detailed treatment of the RSD2013 model is considered elsewhere [8].

The target is partitioned in a number of surface cells to spatially resolve both the non-uniform ion current and the redeposition profile. Each surface cell is characterized by its composition defined by three fractions: the metal fraction θ_{m}, the chemisorbed fraction θ_{c} and the compound fraction θ_{r}. The metal fraction θ_{m} is the portion of the target cell that consists of non-reacted metal particles M. The chemisorbed fraction θ_{c} and the compound fraction θ_{r} are the portions of reacted metal particles MR_z respectively formed by chemisorption of reactive gas at the surface and by reaction with implanted reactive gas atoms in the subsurface. A unique stoichiometry z of the reacted particles is supposed. Due to erosion of the target, the compound fraction formed below the surface is transported to the surface. The inclusion of reactive ion implantation and the reaction of these implanted species with non-reacted metal below the target surface asks for an in-depth partitioning of the target over the implantation range in subsurface cells. A subsurface cell is then specified by the concentration n_{M} of non-reacted metal and by the concentration n_{R} of unbounded implanted reactive gas atoms. As a constant density n_0 of metal atoms is assumed, independent of its chemical state, the concentration n_{MR_z} of compound particles directly follows as:

$$n_{\mathrm{MR}_z} = n_0 - n_{\mathrm{M}}. \tag{1}$$

In the time formulation of the RSD2013 model, the fractions θ_{m}, θ_{c} and θ_{r} of each target surface cell are each described by an ordinary differential equation (ODE). The derivation of these ODEs has been treated before [8]. Here the equations are just given for completeness:

$$\begin{aligned} n_{0,\mathrm{s}}\frac{\mathrm{d}\theta_{\mathrm{m}}}{\mathrm{d}t} &= jY_{\mathrm{av}}(1-\theta_b) - jY_{\mathrm{m}}\theta_{\mathrm{m}} - (F_{\mathrm{m}}+F_{\mathrm{r}})\theta_{\mathrm{m}} + F_{\mathrm{m}} + j\frac{\beta}{z}\theta_{\mathrm{c}} \\ &\quad - F\frac{2}{z}\alpha_t\theta_{\mathrm{m}} \end{aligned} \tag{2}$$

$$n_{0,\mathrm{s}}\frac{\mathrm{d}\theta_{\mathrm{r}}}{\mathrm{d}t} = jY_{\mathrm{av}}\theta_b - jY_{\mathrm{r}}\theta_{\mathrm{r}} - (F_{\mathrm{m}}+F_{\mathrm{r}})\theta_{\mathrm{r}} + F_{\mathrm{r}} \tag{3}$$

$$n_{0,\mathrm{s}}\frac{\mathrm{d}\theta_{\mathrm{c}}}{\mathrm{d}t} = -jY_{\mathrm{c}}\theta_{\mathrm{c}} - (F_{\mathrm{m}}+F_{\mathrm{r}})\theta_{\mathrm{c}} - j\frac{\beta}{z}\theta_{\mathrm{c}} + F\frac{2}{z}\alpha_t\theta_{\mathrm{m}}. \tag{4}$$

The fluxes F_{m} and F_{r} are respectively the flux of redeposited non-reacted and reacted metal which are defined as

$$F_{\mathrm{m}} = \varepsilon_t\frac{I_{\mathrm{tot}}}{A_t}Y_{\mathrm{m}}\overline{\theta_{\mathrm{m}}} \tag{5}$$

$$F_{\mathrm{r}} = \varepsilon_t\frac{I_{\mathrm{tot}}}{A_t}(Y_{\mathrm{r}}\overline{\theta_{\mathrm{r}}} + Y_{\mathrm{c}}\overline{\theta_{\mathrm{c}}}). \tag{6}$$

or stated differently, they are defined by the fraction of sputtered material returning to the target. The fraction variables $\overline{\theta_{\mathrm{m}}}$, $\overline{\theta_{\mathrm{r}}}$ and $\overline{\theta_{\mathrm{c}}}$ are averages over all surface cells weighted with their local ion current. In Eqs. (2)–(6), there are three cell depended parameters: the ion current density j, the area A_{t} and the redeposition fraction ε_t. The total redeposition fraction E_t is the sum of all these individual redeposition fractions ε_t.

The model describes both the sputtering and the returning of the reacted particles as MR_z species. As shown by Berg et al. [11], the difference between an atomic and molecular approach is small but in that case redeposition was not included. As the radial profiles of both the sputtered metal and oxygen atoms are similar, the discussion narrows to the difference in return probability. The latter is due to its low mass normally higher for oxygen as compared to the metal. This can induce faster oxidation of the target but the effect will be small in metallic mode, because little compound is present on the target. In poisoned mode, the effect is even smaller because the returning atomic oxygen cannot stick on the target, and the returning metal atoms will be easily converted to compound due to the high oxygen partial pressure. Summarizing, also in the case of redeposition, we expect small differences between an atomic and a molecular approach.

The average sputter yield Y_{av} is also a cell dependent variable, as it is a weighted average of the sputter yields with the cell specific composition fractions. It is given as

$$Y_{\mathrm{av}} = Y_{\mathrm{m}}\theta_{\mathrm{m}} + Y_{\mathrm{c}}\theta_{\mathrm{c}} + Y_{\mathrm{r}}\theta_{\mathrm{r}} \tag{7}$$