Applying "The Upgraded Berg Model" to Predict Hysteresis Free Reactive Sputtering

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ABSTRACT

Reactive sputtering is a popular process to deposit oxides, nitrides, and several other compounds. Unfortunately, this process mostly exhibits a hysteresis effect. The hysteresis causes a delicate choice of either a high deposition rate but not a fully oxidised/nitrided film or a fully formed compound film but at a significantly lower deposition rate. For high reactivity target material/reactive gas systems, the hysteresis forces the process to flip quite abruptly between these two conditions. Process control may therefore be quite critical. In this work we will use the original "Berg model" as well as the newly published "upgraded Berg model" to illustrate how hysteresis is generated. We have selected one simple graph (reactive gas flow vs. partial pressure) that gives clear indications of how the process may be affected in such a way as to decrease or even eliminate the hysteresis. Specific values of target size and composition, gas mixture as well as total pressure and pumping speed are processing parameters that may be selected in a way to eliminate hysteresis. We will show that this behaviour is predicted by the "upgraded Berg model" and also show experimental evidence for such behaviour.

INTRODUCTION

Reactive magnetron sputtering is one of the most widely used techniques for deposition of thin films. Compound thin films are synthesized by sputtering from a target made of metal, alloy or compound in the presence of a reactive gas. In this process, it is possible to tune the film composition from pure metal to stoichiometric compound by changing the supply of a reactive gas (e.g. oxygen) when sputtering from a metallic target. By using different combination of target material and reactive gas, it is therefore possible to deposit a wide variety of compounds (oxides, nitrides, carbides, sulphides, etc.) with a wide range of properties. This versatility makes reactive sputtering one of the most widely used industrial thin film deposition processes. A drawback with the reactive sputtering process is that the relationship between the reactive gas supply and film composition is normally very non-linear and highly complex and often exhibiting a hysteresis effect. The process offers either a high deposition rate of a slightly sub-stoichiometric film or a fully stoichiometric film deposited at a significantly lower deposition rate. Therefore, the ability to operate the process smoothly between these conditions requires elimination of the hysteresis.

In this work we will use the original as well as the newly "upgraded Berg model" to illustrate some conditions that allow for reduction or even elimination of the hysteresis effect [1-3]. Processing parameters that strongly affect the hysteresis include the size and composition of the target [4-6], gas mixture [7], total processing pressure [8], as well as pumping speed [9, 10]. Proper choice of these parameters may cause the hysteresis to disappear.

THE BASIC MODEL

The original "Berg model" is a quite simple description of the reactive sputtering process. It is based on three analytical equations describing the gas flow balance in the sputtering chamber and material balances at the target and substrate at steady-state conditions [3]. With the original model it is possible to predict results when chemisorption at the target surface is the only compound formation mechanism. Depla and co-workers, however, showed that reactive gas implantation may also play a decisive role for the process behaviour [11, 12]. By introducing this effect, it is possible to extend the original Berg model to also include some additional processing features not possible to describe by the original model. This modified model will be referred to as the upgraded Berg model [2]. The discussions in the following paragraphs are based on the results from [2, 3].

GENERATING PROCESSING GRAPHS

A typical processing curve illustrating the partial pressure of the reactive gas, P_r, vs. the supply of the reactive gas, Q, is shown in Figure 1a.The solid line is the calculated processing curve. The arrows from A to B and C to D indicate the actual processing pathways if the supply Q of the reactive gas is the "control" parameter (=x-axis). The distance between the arrows defines the hysteresis width. Notice that in the hysteresis region there exist three different values (P_1, P_2, and

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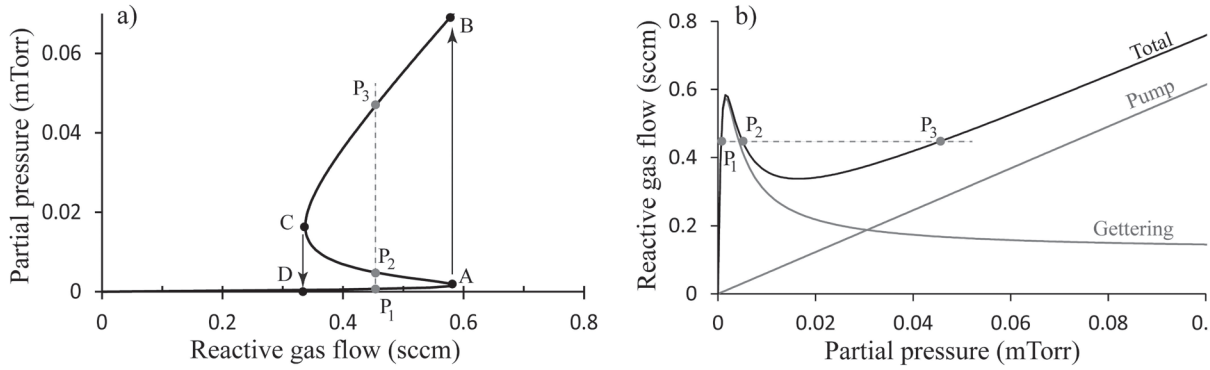

Figure 1: Reactive gas pressure vs. reactive gas flow (a). The reactive gas consumption and its sub-components, i.e. gettering at the chamber surfaces and substrate as well as consumption at the pump, vs. the pressure of reactive gas (b).

P_3) for one value of Q. The curve segment between A and C cannot be reached when the process exhibit hysteresis and is controlled by the reactive gas supply.

The corresponding curve Q vs P_r (Figure 1b), however, has no curve segment with multiple values of Q for one value of Pr. The processing points P_1, P_2, and P_3 are single valued defined for three different values of P_r. This explains why it is possible to obtain a stable process if the partial pressure P_r is chosen as the control parameter instead of the supply, Q, of reactive gas.

The curve representing the total consumption of reactive gas in Figure 1b is the sum of the throughput of reactive gas to the external pump and the gettering of reactive gas when reacting with metal atoms at the substrate and chamber walls. These individual curves are shown as gray lines in Figure 1b. We assume that at steady state conditions all reactive gas forming compound at the target surface will be sputter eroded and again form reactive gas molecules. Therefore there will be no net gettering of the reactive gas at the target surface. What comes in must come out.

The gray straight line represents the throughput of the reactive gas to the external pump and the slope of this line is proportional to the pumping speed. The other gray curve represents the gettering of reactive gas at the substrate surface. This curve has a segment of negative slope. If the maximum value of this negative slope is larger than the value of the positive slope of the straight line the process will exhibit hysteresis. By analyzing this condition for a specific reactive sputtering process it is thus possible to predict if there will be hysteresis or not. In the following we will use the curves in Figure 1b as comparison when altering some key parameter.

FUNDAMENTAL TARGET PROPERTIES

Some processing parameters may be selected by the operator while some others, however, are selected by nature. Examples of the latter are different materials and gas specific properties such as sputtering yields and reactivity.

Reactivity of the Process

In the simulations, a high reactivity process is represented by a high sticking coefficient of the reactive gas onto the sputtered metal. Such a high reactivity process is shown in Figure 1 where the sticking coefficient was set to 1.0. A comparison with this situation and identical processes but with a lower value of the sticking coefficients is shown in Figure 2a-b. As can be seen in Figure 2b the negative slope decreases as the value of the sticking coefficient decreases. This may be explained by the fact that for any given reactive gas flux, cor-

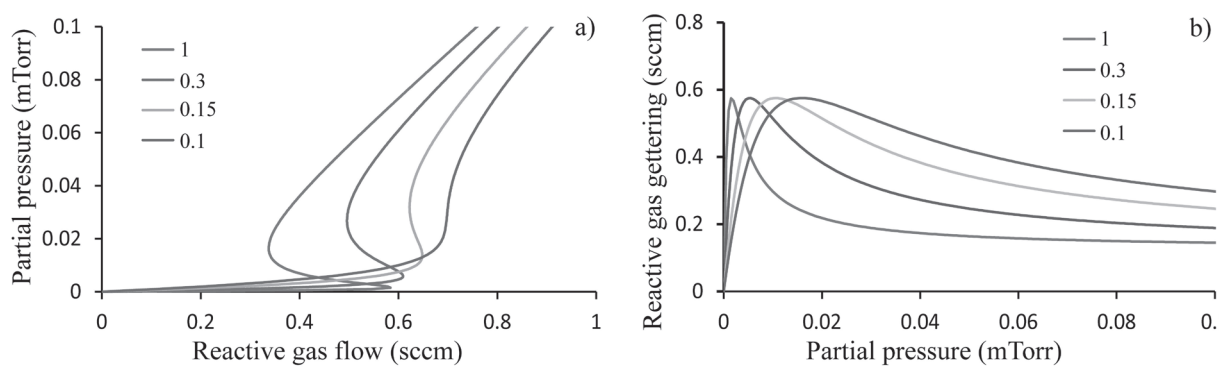

Figure 2: Reactive gas pressure vs. reactive gas flow (a) and substrate reactive gas gettering vs. reactive gas pressure (b) for different sticking coefficients (0.1, 0.15, 0.3, 1.0).

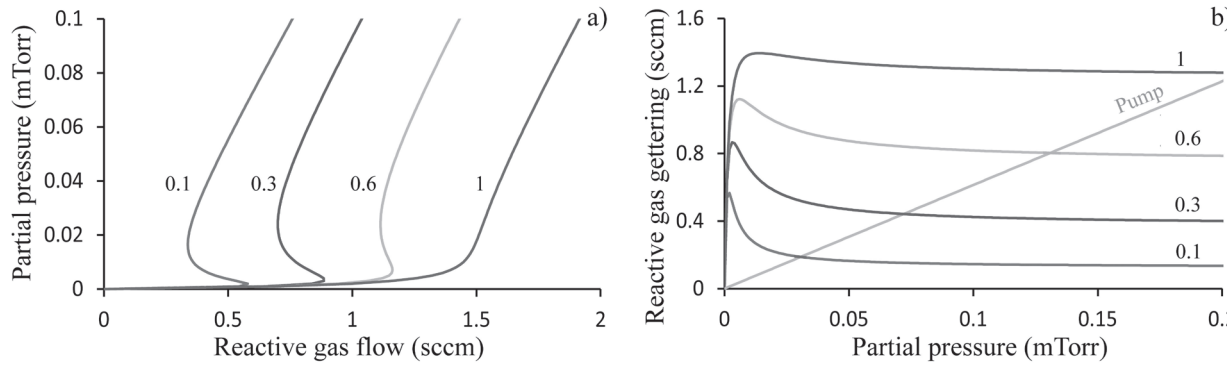

Figure 3: Reactive gas pressure vs. reactive gas flow (a) and pump and substrate reactive gas gettering vs. reactive gas pressure (b) for different compound sputtering yields (0.1, 0.3, 0.6, 1.0) while keeping the metal yield constant at 1.5.

responding to a certain reactive gas pressure, a smaller amount of reactive gas is reacting, i.e. is consumed, at the substrate and chamber walls when the sticking coefficient is reduced. In order to consume the same amount of reactive gas, a higher reactive gas pressure is required for low reactivity systems. This will stretch the curve to the right, i.e. to higher reactive gas pressures and subsequently the slope will be smaller. This leads to a smaller and smaller hysteresis width as the sticking coefficient is reduced and finally a complete absence of hysteresis [13]. The difference in reactivity between oxygen and nitrogen often results in less pronounced hysteresis for nitrides as compared to oxides. This is primarily due to the higher reactivity for oxides.

Sputtering Yields

A reduced yield of the compound material promotes formation of compound at the target surface. The influence on the hysteresis effect from such promoted compound formation is similar to that from a higher reactivity, i.e. the hysteresis width increases. Further, the relative difference between the yields of metal and compound will significantly affect the hysteresis behavior [14]. The metal yield determines the maximum amount that may be consumed at the substrate and chamber walls, i.e. the peak of the corresponding gray curve in Figure 1b. The compound yield, on the other hand, determines the gas consumption at high pressures, i.e. when the curve flattens out. A larger difference between these yields implies a larger difference between the maximum value of the gray curve at low pressure and the leveled out value at high pressures. A large difference between these values implies a larger negative slope of the transition between them and accordingly a more pronounced hysteresis. In Figure 1 the sputtering yield of the compound material was set to 0.1. However, if the sputtering yield of the compound formed at the target surface is closer to the value of the sputtering yield of the metal the value of the negative slope of the gettering curves will decrease. This is illustrated in Figure 3. If this situation is expected one may also expect a less pronounced hysteresis.

INCREASING THE PUMPING SPEED

By increasing the pumping speed from the original value in Figure 1b the new processing curves will be the solid lines in Figure 4. A change in pumping speed will not influence the gettering curve. Only the slope of the straight line, which is proportional to the pumping speed, will be increased. As seen from the figure it will always be possible to increase this slope to a value larger than the maximum negative slope of the substrate gettering curve. The result by increasing the pumping speed sufficiently high is therefore that the new process will not exhibit hysteresis. Experimentally this was first reported by Serikawa and Okamoto [9].

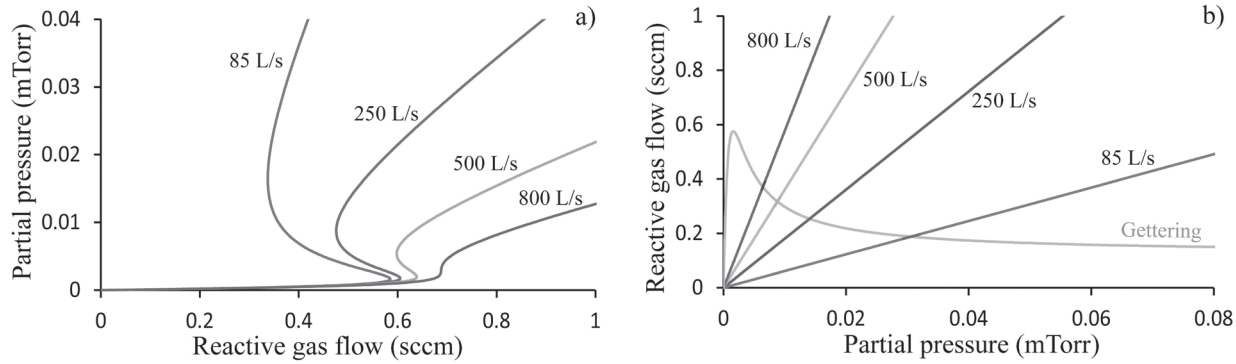

Figure 4: Reactive gas pressure vs. reactive gas flow (a) and reactive gas consumed by the pump and the substrate surface vs. reactive gas pressure (b) for different pumping speeds (85 L/s, 250 L/s, 500 L/s, 800 L/s).

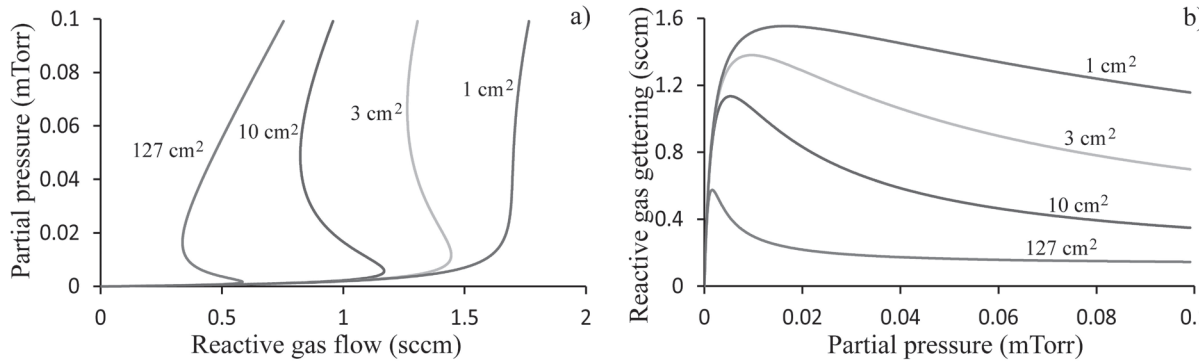

Figure 5: Reactive gas pressure vs. reactive gas flow (a) and substrate reactive gas gettering vs. reactive gas pressure (b) for different target erosion areas (1 cm2, 3 cm2, 10 cm2, 127 cm2).

DECREASING THE TARGET SIZE

By decreasing the target size while keeping the target current constant, the negative slope of the gettering curve will decrease. It should be pointed out that this effect is not achieved if the current density is increased by means of increasing the total target current (keeping the same target area). An increased total current will increase both the maximum value of the gettering curve as well as the level at high pressures, resulting in no difference in the negative slope. However, a constant current and a smaller target area result in an increased maximum value as well as a stretching of the curve towards higher pressures, resulting in a reduced negative slope and thereby a less pronounced hysteresis. Consequently, a reduced target area makes it possible to obtain conditions where this negative slope will be smaller than the slope of the throughput of the pump. Calculated curves for such conditions are shown in Figure 5 and it is seen that the resulting processing curve does not exhibit any hysteresis. This was experimentally verified by Nyberg et. al. [5].

REACTIVE SPUTTERING WITH AN EXTRA REACTIVE GAS

Carrying out reactive sputtering with a metal target and a varying supply of oxygen in the presence of a constant supply of nitrogen may also result in a hysteresis free process. The much more reactive oxygen will replace the less reactive nitrogen bonded to the metal. This has been shown experimentally by Severin et. al. [7]. It should be mentioned that despite quite some nitrogen present in the chamber the deposited film may contain very little nitrogen. The reason for this is that unreacted metal atoms exposed to a mixture of oxygen and nitrogen will initially form chemical bonds with the arriving atoms in approximate proportion to their fluxes multiplied by their reactivities. After some time, reactive gas molecules will arrive at already reacted metal atoms. When oxygen arrives onto nitrided parts, a substitution with nitrogen will occur and all metal atoms will finally be oxidized.

REACTIVE SPUTTERING FROM A PARTLY MIXED TARGET

A target that contains a conducting uniform mix of metal and its corresponding oxide may also give rise to a hysteresis free processing curve. Also here the negative slope decreases as the fraction of oxide in the target increases. As a result the value of the negative slope will be smaller than the slope of the throughput of the pump resulting in elimination of the hysteresis. The introduction of a compound part in the target results in a less reactive system and hence a reduced hysteresis. The overall erosion rate is however smaller as compared to a metallic target. Experimental evidence of this behavior has been shown by Kubart et al. using a mixed TiO_x target [4] and by Särhammar et al. using a target consisting of segments of metal and corresponding oxide for a number of different metals [6].

The results in the abvove two paragraphs can be understood by the effect of difference in sputter erosion of the metal from the target at low supply of reactive gas and from the fully poisoned target as discussed in the "Fundamental Target Properties" paragraph above. The processing condition in both cases starts from a partly “poisoned” target. Therefore the erosion rate ratio from “metal” state to poisoned state is reduced as compared to that of a pure metal.

INCREASING THE ARGON PRESSURE

The poisoning of the target will take place by two different processes.

i) Chemisorption at the target surface due to reactions between the flux of incoming neutral reactive gas molecules and the target metal.
ii) Implantation of ionized reactive gas molecules hitting the target with the full target potential and reacting with metal atoms some distance beneath the target surface.

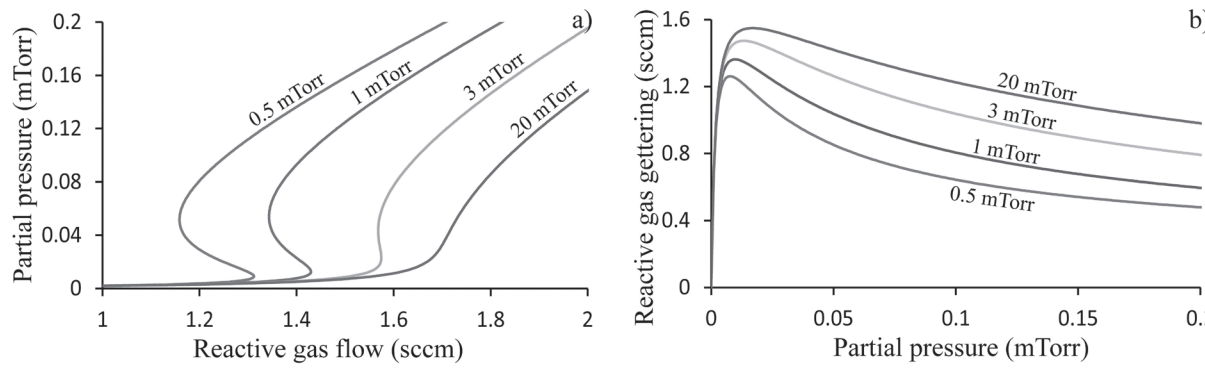

Figure 6: Reactive gas pressure vs. reactive gas flow (a) and substrate reactive gas gettering vs. reactive gas pressure (b) for different processing pressures (0.5 mTorr, 1 mTorr, 3 mTorr, 20 mTorr).

The implantation effect depends on the fraction of target current that is carried by reactive gas ions. This may roughly be approximated by the ratio between the partial pressure of the reactive gas and the total pressure. At high argon pressures, this ratio is negligible while it may be substantial at lower argon pressures. Chemisorption, on the other hand, only depends on the reactive gas partial pressure and is consequently not influenced by the total processing pressure. Since the chemisorption is independent and ion implantation scales inversely with the processing pressure, it is possible to substantially reduce the effect of ion implantation by increasing the pressure, thus leaving chemisorption as the dominating target poisoning mechanism. In the original Berg model, it was assumed that the only poisoning mechanism was chemisorption. To account for the pressure dependent effects described here, also the implantation effect has to be accounted for [2].

Simulations based on the upgraded Berg model are shown in Figure 6. It is seen that the hysteresis may be eliminated at higher processing pressures. This has also been confirmed by experiments [8]. This finds its origin in the interplay between the two poisoning mechanisms of the target described above. At low pressures both chemisorption and ion implantation are responsible for target poisoning while at high pressures, only chemisorption is present. This corresponds to a high reactivity system (implying large hysteresis) at low pressure and less reactive system at high pressures (implying less hysteresis). If the sticking coefficient for chemisorption is not sufficiently high to cause hysteresis alone, the process is hysteresis-free at high pressures but may have a substantial hysteresis at lower pressures. On the other hand, if the chemisorption coefficient is large enough to give rise to hysteresis alone, the process will exhibit hysteresis throughout the pressure range, albeit a somewhat larger hysteresis at lower pressures.

CONCLUSION

By applying quite simple process modelling it is possible to obtain indications on how to adjust the involved parameters to decrease or even eliminate the hysteresis for reactive sputtering processes. The examples above hopefully illustrate this. We believe that there are most probably more processing parameters and features than the ones reported here that may affect the hysteresis. We will continue to search for other conditions that allow for elimination of hysteresis in the reactive sputtering process.

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