Contents lists available at ScienceDirect

Surface & Coatings Technology

Applying "the upgraded Berg model" to predict hysteresis free reactive sputtering☆

E. Särhammar, T. Nyberg *, S. Berg

The Ångström Laboratory, Solid State Electronics, P.O. Box 534, SE-751 21 Uppsala, Sweden

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 oxidized/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 abrupt 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 behavior is predicted by the simulations and also refer to experimental evidence for such behavior.

© 2016 Published by Elsevier B.V.

1. 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, sulfides, 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.

2. 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 behavior [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 be described by the original model. This modified model will be referred to as the upgraded Berg model [2] and is only used in Section 9 which treats the influence from the total processing pressure on the hysteresis effect. Both models are kept as simple as possible and may be used to illustrate general trends and influences from different parameters. Therefore, small deviations between the simulated values and absolute experimental values may occur. For instance, the partial pressure in metal mode is normally somewhat
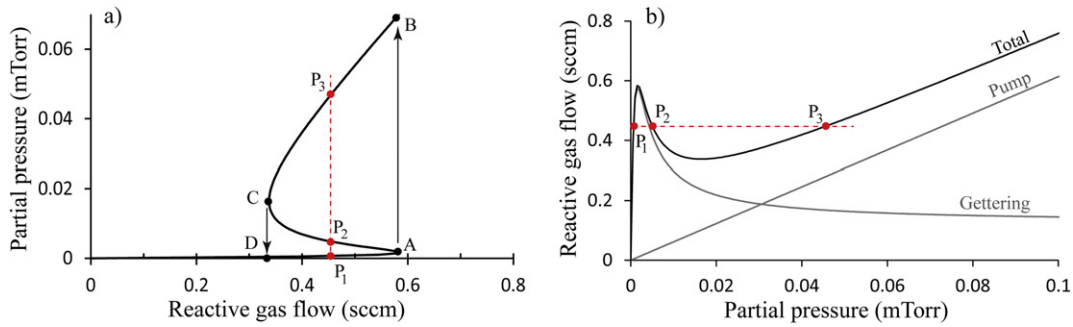
Fig. 1. Reactive gas pressure vs. reactive gas flow (a). The reactive gas flow and its sub-components, i.e. gettering at the chamber surfaces and substrate as well as consumption at the pump vs. the pressure of reactive gas (b).

lower in the simulations as compared to experiments. The discussions in the following paragraphs are based on the results from references [2] and [3].

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 Fig. 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 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 (Fig. 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 Fig. 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 Fig. 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 Fig. 1b as comparison when altering some key parameter.

4. 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.

4.1. 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 Fig. 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 Fig. 2a—b. As can be seen in Fig. 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, corresponding 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.
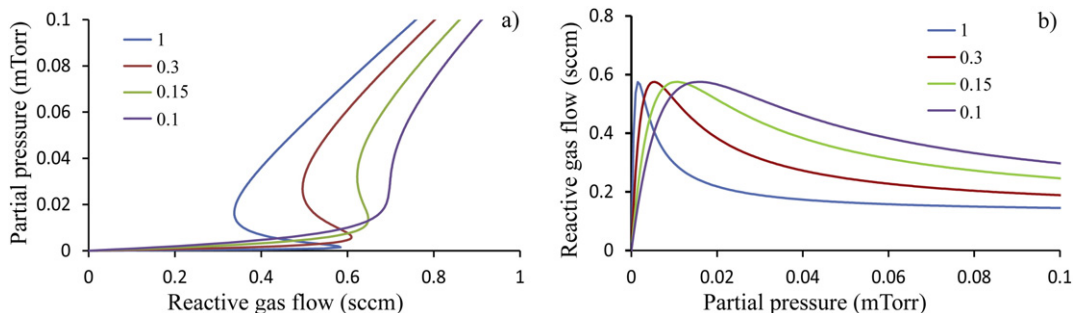

Fig. 2. Reactive gas pressure vs. reactive gas flow (a) and reactive gas flow vs. reactive gas pressure (b) for different sticking coefficients (0.1, 0.15, 0.3, 1.0).