Workshop on Sputtering
Room Constellation C, Hyatt Regency - Session WS-SuM
Workshop on Sputtering (Morning Session)

Moderator: W.D. Sproul, Advanced Energy Industries, Inc.

10:00am **WS-SuM1 Basic Understanding of Reactive Sputtering Processes*,* *S. Berg*, *T. Nyberg,* Uppsala University, Sweden **INVITED**

Reactive sputtering is a mixed physical and chemical vapour deposition process. It is frequently used in a wide variety of industrial applications. It is not, however, a simple matter to combine high rate reactive sputter deposition and process stability. The reactive gas may easily poison the target causing the deposition rate to decrease sometimes as much as a 5-20 times. In addition the process exhibits a hysteresis behaviour in the relations between the primary processing parameters. In a large volume production situation this may cause serious problems. There must be some sort of built in control system to force the process to avoid being trapped in the hysteresis loop and entering too far into the target poisoned mode. Process modeling of the reactive sputtering process may serve to illustrate the influence of different processing parameters on the overall behaviour of the process. A quite successful model for the basic behaviour of the reactive sputtering process have been suggested by Berg and co-workers. It is frequently referred to as Berg´s model. This model enables to predict the general shapes of most experimental reactive sputtering processing observations. It may predict the complex realations between the partial pressure and supply of the reactive gas as well as the fraction of target poisoning and the composition and deposition rate of the growing film. Knowing the actual relations between these parameters significantly assists in designing reliable control systems for reactive sputtering processes. A detailed analysis suggests that there exist several ways of eliminating the hysteresis in reactive sputtering processes. Increasing the pumping speed of the system will ultimately result in elimination of the hysteresis. Decreasing the effective sputter erosion zone at the target may also result in elimination of the hystereis. Hysteresis or no hysteresis depend on a critical balance between the gettering of the reactive gas by compound formation of the growing film and the amount of the supplied reactive gas eliminated from the processing chamber by the external pump. There exists several ways of "twisting and turning" this balance. This will be shown in this presentation. Sputtering from more than one target (co-sputtering of different elements) and/or the use of more than one reactive gas in a reactive sputtering process will significantly increase the complexity of the process. Reproducing deposition rate and film composition under such conditions may be hazardous. Input processing parameters interact with each other in such a way that not only their absolute values are important but also the sequence in wich that they are varied must be taken into account. This makes process control quite problematic. We will illustrate how such conditions occur and suggest how to be in full control of the process. @FootnoteText@ 1. Computer modeling as a tool to predict deposition rate and film composition in the reactive sputtering process.: S. Berg, T.Nyberg, H-O.Blom and C.Nender; J.Vac.Sci.Technol.A16(3)May/June 1998,p1277-85 2. Modeling of the reactive sputtering process: S. Berg, T.Nyberg, H-O.Blom and C.Nender Handbook of thin film process technology, Edited by D.A.Glocker and S.I.Shah, Inst.of Physics, 1998, pp A5.3:1-15 3. Review article to appear in the journal Thin Solid Films in spring 2004.

11:00am **WS-SuM3 Shallow Implantation as a Mechanism for Target Poisoning in Reactive Sputtering*,* *R. De Gryse*, *D. Depla, J. Haemers, G. Buyle,* University Ghent, Belgium **INVITED**

Up to now, reactive sputtering and in particular the target poisoning effect has been described in terms of gettering and chemisorption. It is modelled by a set of linear differential equations@footnote 1@ which predict the non linear poisoning behaviour as a function of the mole fraction of the reactive gas (RG). From this picture it also follows that a decrease in sputter rate as well as a decrease in absolute target voltage (ATV) is expected. The expected decrease in ATV relies on the fact that it is widely accepted that the ion induced secondary electron emission coefficient (ISEE) of compounds is larger as compared to the ISEE of the corresponding metal. However, the experiment shows that several combinations of metal - (R.G.) give rise to an increase in ATV upon poisoning. In systems such as Nb/O@sub 2@@footnote 2@; Sn/O@sub 2@@footnote 2@;Si/N@sub 2@; etc. the ATV is reported to increase when poisoning occurs. Recently it has been suggested that the poisoning instability is not always due to the chemisorption effect but can also be ascribed to the combined effect of target etching, preferential sputtering of metal vis a vis compound and shallow implantation of reaction gas into the target near surface region. This D.R.@footnote 3@ model also leads to a poisoning instability without any need of wall gettering and also two levels in sputtering speed depending on the fraction of (RG) i.e. a high sputtering speed for low mole fractions and a low sputtering speed for higher mole fractions. This behaviour has been simulated by means of the TRIDYN code.@footnote 4@. The transition between metallic and compound or poisoned regime can be predicted as a function of an experimental parameter which contains quantities such as pumping speed, wall area, discharge current, sputter efficiency etc. In this model it is assumed, and shown experimentally, that non bonded RG can be present in a shallow surface layer. It is also shown that this non bonded RG is a component which can give rise to an increase in ATV upon poisoning. Also chemisorption, if present, can give rise to an increase in ATV. Reality will probably be best modelled by a combination of the gettering model and the D.R. model.@footnote 5@ In metallic mode, the magnetron discharge can be described quite accurately and several tools are at our disposal varying from Analytical models over Fluid models, Boltzmann models, Monte Carlo models/Particle in cell (MC-PIC) models to Hybrid models (MC-Fluid). All these models are in some or other way a trade off between speed and accuracy. However in pure metallic sputtering the accuracy and speed of the analytical approach is surprising.@footnote 6@ Modelling of the magnetron discharge in poisoned or compound mode requires the correct picture of the poisoning mechanism. This will allow to predict over the full range of reactive gas flows quantities such as number densities, energy and directivity of the different material fluxes towards the substrate. This in turn will give an estimate of the expected deposition speeds, coating homogeneity, target consumption and will eventually predict the growth mechanism of the coating. The ultimate goal is to develop for every particular application a stable running magnetron. @FootnoteText@ @footnote 1@S. Berg et al., J. Vac. Sc. Technol. A5(2), 1987, p. 202. @footnote 2@"Sputter Deposition" by W. Westwood ISBN 0-7354-0105-5. @footnote 3@D. Depla et al., Vacuum 66 (2002) p. 9. @footnote 4@Z.Y. Chen et al., Nucl. Instr. Meth. In Physd. Res. B: in press. @footnote 5@D. Depla, R. De Gryse, submitted for publication in Surface and Coatings Technology. @footnote 6@G. Buyle et al., J. Vac. Sci. Technol., A21(4), July/August 2003.

11:40am **WS-SuM5 Modeling of Sputtering Equipment and Processes as an Engineering Tool: Building a Virtual Sputter Tool*,* *J.C.S. Kools,*** Veeco Instruments **INVITED**

In recent years, computational modeling has emerged as an attractive engineering tool to substantially reduce the development time and cost for both equipment and process development of industrial thin film deposition and etch. Furthermore, due to the dramatic increase in computing power available, advanced computational techniques such as Molecular Dynamics have migrated from the academic community to the engineering community, bringing more realistic models within its reach. Our goal is to build a "virtual sputter tool" that could predict the sputter equipment behavior and film properties. Fig.1 sketches the outline of a virtual sputter tool. As can be seen, such a Multiscale/Multiphysics model comprises both advanced computational techniques, such as Particle-In-Cell Monte-Carlo (PIC-MC) and conventional continuum descriptions such as Finite Element Analysis (FEA). In this talk, we will review the progress that has been made towards building a virtual sputter tool, comparing modeling and experimental results. We will put most emphasis on the right hand side of the diagram, namely the modeling of film properties, in the context of industrial application. We will discuss the future outlook towards completion of the virtual sputter tool.

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