

THE REACTIVE SPUTTER MODEL RSD2013

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For a realistic description of the growth and the structure formation of a thin film, it is vital to have accurate knowledge of the arriving species at the substrate level. In the case of reactive magnetron sputter deposition, the origin and characteristics of these deposited species are tightly connected to the state of the sputtered target, and therefore it is not surprising that the growth mechanisms during reactive sputtering is defined by the target condition. Depending on the tunable operation conditions, the target will be sputtering in a metallic, a poisoned or an unstable transitional state. The states are in essence defined by the fraction of the target that is transformed from a metallic surface to a compound surface. Retrieving in an experimental way information on the target condition is difficult as most deposition parameters are connected to the average target condition. Moreover, despite the practical simplicity of the deposition technique, its underlying physics is complex and non-linear due to a hysteresis phenomena which is characteristic for the process. Here simulations can play a key role. The simulation tool RSD2013 enables us to simulate the DC reactive sputter process as function of practical adjustable parameters. As the improved RSD model is capable to simulate in detail the target condition as function of the experimental conditions, it paves the way for a deeper understanding of the influence of the deposition condition on the film growth. In the RSD model the change of the target condition from the metallic to the poisoned state is performed by including mainly three target processes: the chemisorption of reactive gas species, direct and knock-on implantation of reactive species and the redeposition of sputtered material. Both the state of the target and the substrates are described in a spatial resolved way. The proposed equations can as well be solved in a time dependent as in steady state way. During its development, specific attention was given to connect the code to other simulation tools such as the Monte-Carlo codes SIMTRA, for the transport of the sputtered species, and SRIM, for the ion-target interactions. This connection results in a strong simulation package which allows to get detailed information on the target condition. In this paper, the capabilities of this simulation package will be elucidated with some well-chosen examples, focusing on the fundamental understanding of this PVD technique, and to the relation between the target condition and the film growth.