Modeling the time dependency of the reactive sputter process

Abstract

Simulation results of a developed non-stationary RSD (Reactive Sputter Deposition) model are presented. The basis principles of the model come from a stationary version which was already applied in earlier work [1], and which was further developed. Both models, the stationary and the non-stationary, include the following poisoning mechanisms: chemisorption, direct and knock-on reactive ion implantation. The models are reinforced with the ability of including a deposition profile on the substrate, a redeposition profile on the target, a non-uniform ion current and an analytical plasma model [2] of the DC discharge. Combined with the SIMTRA package [3] and SRIM [4], this gives us a strong tool to investigate the time evolution and the mechanisms of the target poisoning.

Capabilities of the model

Simulation results of a developed non-stationary RSD (Reactive Sputter Deposition) model are presented. The basis principles of the model come from a stationary version which was already applied in earlier work [1], and which was further developed. Both models, the stationary and the non-stationary, include the following poisoning mechanisms: chemisorption, direct and knock-on reactive ion implantation. The models are reinforced with the ability of including a deposition profile on the substrate, a redeposition profile on the target, a non-uniform ion current and an analytical plasma model [2] of the DC discharge. Combined with the SIMTRA package [3] and SRIM [4], this gives us a strong tool to investigate the time evolution and the mechanisms of the target poisoning.

Inert gas pressure influence

Recent work [5] shows the elimination of the hysteresis for low reactivity combination of reactive gas and target material, like Al and O₂, when increasing the inert gas pressure (Ar).

In that work [5] the single-cell stationary RSD model is able to qualitatively reproduce this behavior. Now moving on to a multi-cell description, shown in the left figure, where a non-uniform current is used. A substantial shift of the critical points to higher oxygen flows is observed. The elimination of the hysteresis in function of the Ar pressure is also stronger compared to the single-cell (uniform) case.

Parameters sets for these simulations are comparable as those used in [5]. The current profile is constant and based on a measured erosion profile after long-time sputtering in non-reactive mode. The right figure compares the multi-cell description when considering a redeposition profile (dashed lines), based on SIMTRA simulations, and without the redeposition (full lines). Redeposition will increase with increasing Ar pressure. SIMTRA confirms this behavior with redeposition fractions ranging from 6% to 14% to 28% to 47% for increasing Ar pressure.

Capsabilities of the model

Overview of the present options in the RSD model, with the following restrictions:
1. enabling Current profile disables Redeposition on target
2. enabling Plasma model disables Current profile
3. enforces equal sputter yields for the chemisorbed and the reacted compound

When a Current profile is enabled, the model will adapt a multi-cell description of the target, while a single-cell description for Uniform current

Target poisoning

On the left figure the depth profiles of the target is shown at some selected oxygen flows during a hysteresis simulation in time. The increasing erosion is due to the longer sputter time. The flowpoints in the legend are in chronological order.

The gridding on the figure shows the number of simulation cells and their size. The upper and lower lines delimit the simulated target depth.

The right figure illustrates the metallic fraction at the target surface at the corresponding points of the left figure. It shows the case with and without redeposition. For comparative reasons the current profile and the redeposition profile are added. The faster poisoning of the targets edges is nicely illustrated in the no redeposition case. Redeposition seems to decrease this effect.

Including plasma model

In this figure the influence of a stationary plasma model [2] is illustrated, where the parameters are taken from [2]. The output of the plasma model is a more realistic ratio of reactive to inert ions, compared to the original model ratio used in the RSD model. The simulations should be performed within the single-cell description as the plasma model itself is also unresolved in space.

The no plasma case is compared with the stationary and the non-stationary solution of the RSD model, both with the stationary plasma model enabled. Using a stationary plasma model for the time dependent RSD model is sustained by the much shorter timescale on which the plasma evolves. The correspondence between the two plasma solutions additionally support this claim.

Conclusion

» As the non-uniformity of the current has a dramatic impact on the hysteresis curve, it should not be omitted in future RSD models.
» As such a plasma model for a multi-cell description is highly desired.
» The non-uniform poisoning of the target surface is illustrated.

References