Modeling Of Deposition Processes From Molten Salts

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The temporal discretized Potential Model with moving boundary conditions [1] has been successfully used for modeling direct current plating procedures and etching procedures from/in aqueous solutions. Furthermore, it was used to optimize the parameters for pulse reverse plating (PRP) processes. It will be demonstrated in this contribution, that it allows for a description of deposition processes from molten salts, too. This fact is not really surprising, since the potential model is derived from the complete transport equation (which contains contributions of migration, convection and diffusion, respectively) under the assumption of vanishing concentration gradients. Because of the very high temperature in molten salt electrolytes, concentration gradients equilibrate very fast and this model-assumption seems to be justified.

As an example, the deposition process of titanium diboride (TiB_2) on suitable substrates is modeled under the assumption of secondary current density distributions, i. e. the kinetic resistance of the interfacial reaction is considered to be *not* negligible compared to the ohmic resistance (i. e. a non-zero Wagner number is assumed). A linear current density/overpotential relation with slopes derived from the experimental polarization curve has been used to model the charge transfer polarization behavior. From the comparison of the computed deposition profile with the experimental layer-thickness distribution it turned out, that - in the case of TiB_2 deposition processes - the Potential Model yields excellent results when assuming secondary current density distributions. Since, up to now, only a 2-dimensional numerical solver for the potential model is accessible to our working group, representative cuts (longitudinal cut and cross-section) have been used to evaluate the current density distribution and the layer-thickness distribution on some simple geometries of the substrate. For instance, Fig. 1 shows the current density distribution along a very thin strip with rectangle cross-section (longitudinal cut). Corresponding to the values given in Fig. 1, the current density distribution and layer-thickness distribution has been computed for some selected cross-sections (experimentally verified by cutting the working piece at different positions). It can be seen from Fig. 2 that the agreement between the modeling results and the experimental shapes is a very good one. Since a 3-dimensional numerical solver for the Potential model has been developed recently [1], plating of more complex-shaped working pieces can be modeled in future, too. It has to be noted, that the reaction mechanism for the deposition of TiB_2 is complicated and investigations of the deposit-structure as a function of the applied current densities have to be performed. Since the deposit-structure can be influenced by using pulsed current techniques, modeling of the deposition process with transient signals are currently under investigation.

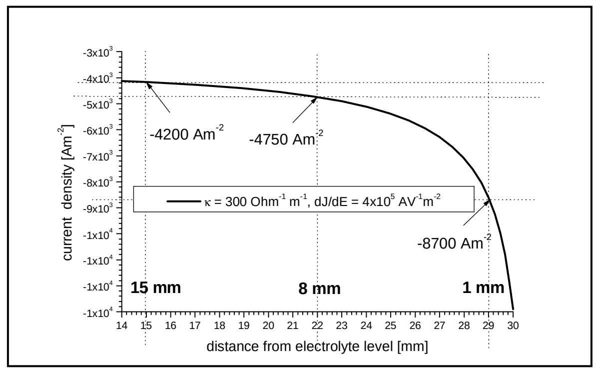

Fig. 1. Current density distribution along a thin strip with rectangle cross-section

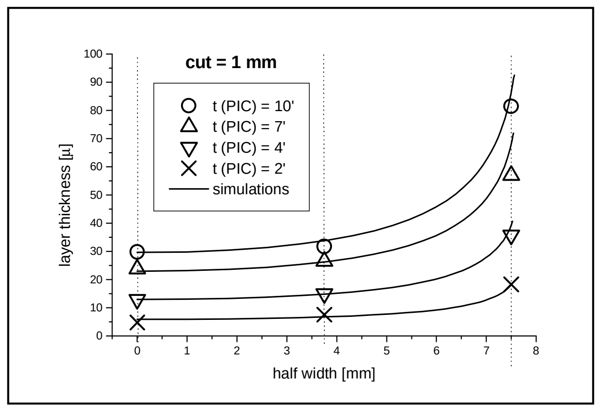

Fig. 2. Layer-thickness distribution along a selected cross-section at different plating times

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