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Predicting Properties of Sputtered Films Directly From Basic Chamber and Process Parameters – Initial Results

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Lack of detailed knowledge of process conditions remains a key challenge in magnetron sputtering, both for chamber design and for process development. Fundamental information such as the pressure and temperature distribution of the sputter gas, and the energies and arrival angles of the sputtered atoms and other energetic species is often missing, or is only estimated from general formulas. However, open-source or low-cost tools are available for modeling the key physics steps of magnetron sputter deposition, which can give more accurate data from desktop computations than traditional empirical approaches.

To get a better understanding of magnetron sputtering, we have collected existing models for the 4 major process steps: dynamics of the plasma using Particle In Cell-Monte Carlo Collision (PIC-MCC), impact of ions on the target using molecular dynamics (MD), transport of sputtered atoms and neutrals in the gas phase using Direct Simulation Monte Carlo (DSMC), and growth of the film using a combination of Kinetic Monte Carlo (KMC) and MD methods. Models have been tested against experimental measurements. For example, the gas rarefaction in front of a magnetron observed by Rossnagel[1] and others has been approximately reproduced, and along with it the models predict a local pressure increase of ~50% which may strongly influence film stress. Results on energies and arrival angles of sputtered atoms and reflected gas neutrals are applied to the KMC and MD simulation of film growth. Experimental center/edge thickness variation for Be films is reproduced to about 6%. Comparison of model results to experiments on SiC roughness evolution with thickness will be presented. Application of the models to improving density and microstructure of SiC and Be films, and future prospects for manipulating film properties, will be discussed.

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1 S. M. Rossnagel, Journal of Vacuum Science & Technology A-Vacuum Surfaces & Films **6**, 19 (1988).