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A Practical Sputter Equipment Simulation System For Aluminum Including Surface Diffusion Model

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Abstract

We have developed a practical aluminum sputter deposition system which is composed of a trajectory calculation module using the Monte Carlo(MC) method, a surface diffusion calculation module, and a deposition profile module using a 'modified' QAS(quasi-axis-symmetrical) approximation. In the system, the string model is utilized as the common data structures for simplifying interface. The simulated profiles (after adjustment of surface diffusion coefficient) well agree with the experiments. The surface diffusion model is found indispensable for aluminum. The adjusted surface diffusion coefficient with the activation energy of 12.4(kJ/mole) is found about one million times as large as the bulk at 573K.

1.Introduction: Aluminum deposition processes are generally used in the semiconductor production. The equipment simulation for aluminum is necessary to improve coverage of contact holes efficiently. Sputter deposition models have been developed and practically utilized[1,2]. But these models were unsuitble for the aluminum profile simulation for lack of flow calculation. Aluminum reflow simulation models also have been studied[3,4]. But these models use such as the flow dynamics and molecular dynamics which need much computational resource and are impractical for deposition simulation. The problems are that sputter deposition and surface flow occur simultaneously during the aluminum deposition process ,and therefore aluminum sediment overhangs contact holes and prevents(or shadows) particle trajectories. So, for the first time, we have developed practical sputter simulation system for aluminum calculating alternately surface flow profiles and deposition profiles taking the precise shadow effect into account and have compared the simulation results with the experiments.

2.Model and System: A block diagram of sputtered aluminum profile simulation system is shown in fig.1. The system is composed of these modules. **(1) Trajectory calculation module:** Tajectories of atoms in the sputter equipment are calculated with the Monte Calro method[1]. The energy dependence of collision cross-section is calculated using the hard sphere approximation. **(2) Deposition profile calculation module:** The deposition profiles of contact holes are calculated using modified QAS approximation, as schematized in fig.2. Different from the previous QAS approximation[1], the shadow effect of a trajectory is judged for all of the string points (Xn, Zn). The cross point (Xcr, Ycr) of the trajectory with the Z=Zn plane is calculated. Then if ($Xcr^2 + Ycr^2 > Xn^2$), the trajectory is neglected by the shadow effect, and else the next position of the string point is calculated with the sticking coefficient of 1. These calculations are repeated for all the trajectories which are calculated with the MC method and saved in a file. **(3) Surface diffusion calculation module:** The flow algorithm developed by Leon[5] is applied because it is well suited to the data structures of the string model used in the above profile calculation module. The flow profiles are calculated using surface diffusion theory where aluminum transports on the surface in order to reduce the suface free energy. For the profile calculation of contact holes axis symmetrical approximation is used.

The modules (2) and (3) are repeated utilizing the string model as the common data structures for simplifing interface. The system is incorporated into the sputter deposition simulator 'SimDepo'. In this system, parameters can be optimized using GUI(graphical user interface) as partially shown in fig.3. As the GUI configuration, Motif is adopted which has made the system easy to operate. Using this system the aluminum deposition profiles can be easily simulated by semiconductor process engineers and sputter equipment designers.

3.Results: Simulated profiles of sputter deposited aluminum are compared with the experiments. Fig.4(a) shows an experimental SEM profile at the wafer center of a 1.2 μm wide 1.0 μm deep contact holes on which 1.0 μm thick aluminum is deposited at a pressure of 1.0 Pa and a temperature of 573K and 0.5 μm thick passivation layer is deposited after aluminum deposition. As shown in fig.4(b), a simulation profile (after adjustment of the surface diffusion coefficient) well reproduces the experiment. As a comparison, a calculated profile leaving the surface diffusion out of consideration, as shown in fig.4(c), disagrees with the experiment. The surface diffusion model is found indispensable for aluminum. The simulated bottom coverages also agree with the experiments about 3% accuracy. The time spent on a profile simulation except the trajectory calculation is about 20 minuites using EWS(130MIPS), which is practical enough. The adjusted surface diffusion coefficients are ploted with the temperatures in fig.5(Arrhenious plot). The activation energy of the surface diffusion is found 12.4(KJ/mole). The surface diffusion coefficient is found about one million times as large as the bulk (literal value) at 573K. The result is similar to previous paper by Fujinaga et.al.[6] about BPSG reflow at 850K. The surface diffusion is verified by microscopic simulations using molecular dynamics.

4.Conclusion: We have established the aluminum deposition simulation system. The surface diffusion model is found very important for aluminum deposition profiles. The adjusted surface diffusion coefficient is about one million times as large as the bulk.

References:

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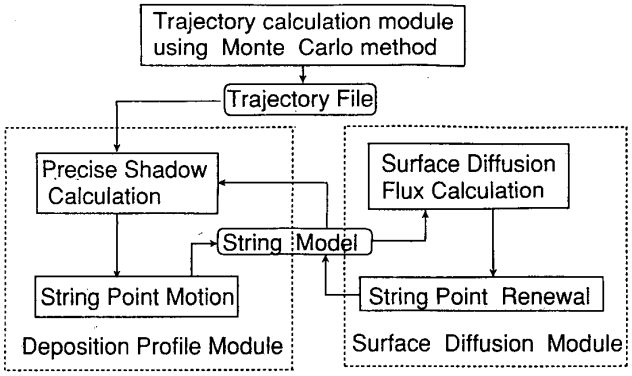


Fig.1 Block Diagram of Aluminum Sputter Simulation System

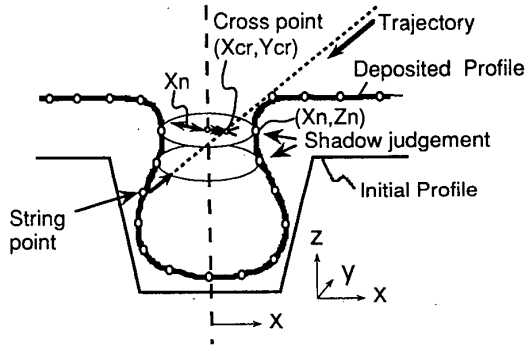


Fig.2 Modified QAS model : Aluminum sediment overhangs contact hole and prevents trajectory. Precise shadow calculation using modified QAS is developed. The string model is utilized.

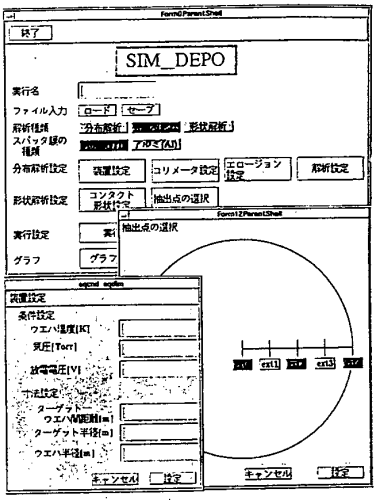


Fig.3 GUI of System (SimDepo)

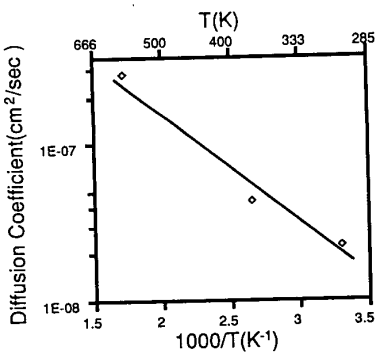


Fig 5. Arrhenious plot

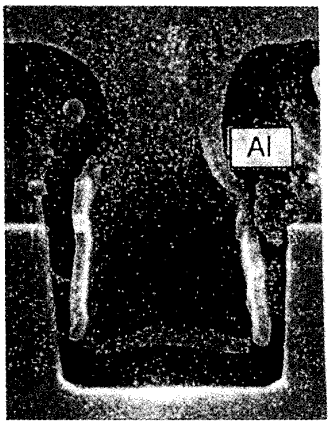
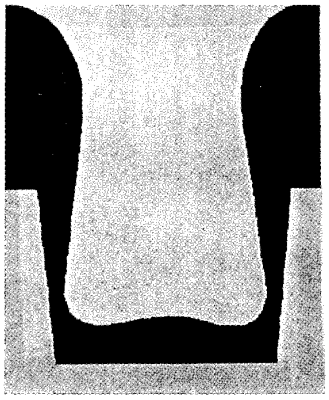


Fig.4(a)Experiment



Fig,4(b)Simulation

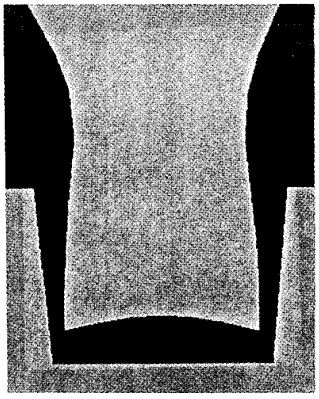


Fig4(c) Simulaion without surface diffusion

Fig.4 Simulated Aluminum Profile and Experiment