Preliminary simulation of Magnetron sputtering using Pegasus software

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In an r.f.-d.c. coupled magnetron sputtering system, the magnetron discharge was generated by a 13.56 MHz r.f. source, and a d.c. power was simultaneously applied to a tin target through a low-pass filter in order to control the incident ion energy on the target. When an extremely low r.f. power 5W and d.c. power sources were applied simultaneously to the target, the glow discharge was about one-seventh of that in the case of the d.c. magnetron discharge.

Keywords – Magnetron discharge, magnetron sputtering, Pegasus software, plasma analysis.

Introduction

Pegasus Software, Inc. developed the plasma, diluted gas analysis software with PEGASUS.

- system design, development, improvement and evaluation;
- development and manufacture of materials and devices;
- prediction of process technology, development and improvement.

Efficiency improvement, support simulator aimed at reducing experimental and prototype cost.

Application scope of PEGASUS

Plasma behavior / neutral particle behavior individually and combined analysis is possible.

- a vacuum apparatus, a CVD apparatus, an etching apparatus, Behavior solution in the magnetron sputtering apparatus Analysis;
- surface modification solution such as ion plating Analysis;
- dry Etching / deposition etc. Table surface shape analysis.

Magnetron sputtering equipment is one of the typical thin-film manufacturing equipment, modeling in a 2-dimensional cylindrical coordinate system.

In this work, simulate the magnetron sputtering device using Pegasus software and analyze it.

Experimental

Module GUI (Graphical User Interface Module; GUIM), should make a preprocessor, post processing and execution of each module of the PEGASUS, PEGASUS for graphical user interface. All the modules of the PEGASUS can be run through this

GUIM.

- calculation criteria, such as species, reactions, Sputtering can be specified by intuitive operation (pre-processor);
- Review results with simple operation, can be considered (post-processor).

Static magnetic field distribution and electron ion density in the device, ion flux and ion energy to the target, flux of sputtered particles jumping out of the target, flux of sputtered particles reaching the substrate, flux of sputtered particles reaching the substrate, etc. are obtained. In this example, we analyze with the following four steps using 4 modules of MSSM, PIC - MCCM, SPUTSM, DSMCM.

1. The static magnetic field created by the magnet is analyzed by MSSM.
2. The state of the plasma in the static magnetic field is analyzed using PIC-MCCM. Ion flux to the
target and the like are obtained.

The PIC-MCCM can analyze the behavior of a non-equilibrium low temperature plasma in an apparatus such as a plasma CVD apparatus, a plasma etching apparatus, a sputtering apparatus, an apparatus for manufacturing a functional thin film, and the plasma density in the apparatus is relatively low $10^{16}$ [#/ m$^3$]; $10^{10}$ [#/ cc] or less) is a module specialized in plasma analysis. It is also possible to analyze charged particle behavior such as electron beam and ion beam trajectory analysis in electromagnetic field.

(3) Using SPUTSM, determine the flux, emission angle distribution, and emission energy of sputtered particles popping out of the target.

SPUTSM is a module that calculates the emission flux, angular distribution, and energy of sputtered particles using SASAMAL with reference to the calculation result of PIC-MCCM (flux of incident ions to the target, energy, incident angle). When conducting sputtering analysis:

- Plasma analysis;
- Evaluation of sputtering rate;
- Analysis is performed by flow such as evaluation of sputtered particles deposited amount on the substrate.

(4) The movement of sputtered particles in the device is tracked by DSMCM and the flux distribution of sputtered particles reaching the substrate is determined.

The DSMCM uses a DSMC method (particle model) such as arranging a large number of sample particles and stopping the collision of these particles stochastically according to a physical model to trace behaviors, and dilution in various vacuum apparatuses. It is a module for analyzing the gas flow field. Kn (number of Knudsen; dimensionless number for evaluating the flow leanness, Kn = length of mean free path length / length of flow representative length) exceeding the application limit of the Navier-Stokes equation that treats gas as a continuum) Is good at analyzing the flow field when Kn > 0.01. It is possible to analyze the behaviors of neutral particles (buffer gas, radical species, sputtering particles) with no charge in etching equipment, thin film manufacturing equipment and sputtering equipment.

Results and discussion

In the following graphs, the temperature, density, production rate of $e^-$, temperature, density and production rate of Ar$^+$ are shown.

Calculation can be performed in the same way by changing the gas pressure (changing the Ar initial density of the PIC-MCCM control parameter), changing the voltage (changing the AC voltage of the electrode setting). Increasing the voltage and gas pressure takes time to reach the steady state, so set the maximum step number to a larger value.

Fig. 2. $e^-$ temperature.

Fig. 3. $e^-$ density.

Fig. 4. $e^-$ production rate.
By using plasma analysis with PIC-MCCM, we calculated the target with tin here and output the waveform of the emission flux distribution of sputtered particles.

Fig. 5. $Ar^+$ temperature

Fig. 6. $Ar^+$ density

Fig. 7. $Ar^+$ production rate

Fig. 8. Total sputte coil.

Fig. 9. Ar sputte coil.

Fig. 10. Sn sputte coil.
In this work, targeting tin ended with a rudimentary simulation. The emission flux of sputtered particles when targeting tin was smaller than the emission flux of sputtered particles of Ar, the waveform output was small. Since a low density target having low thermal conductivity is heated to a high temperature during sputtering, tin monoxide having a high vapor pressure evaporates and is released from the target, and this evaporation molecule is generated in parallel with the sputtered particles. It is thought that it is deposited in the film. Here, it can be easily inferred that the low density target is porous and has a large surface area and promotes the evaporation of the tin component from the low density target.

Simulation of transportation of sputtered particles in Ar gas is carried out by using test particle Monte Carlo method. The sputtered particles flow from the target, fly through the Ar gas, and reach the substrate.

The velocity distribution function of the incoming sputtered particles is obtained from the sputtering simulation. The film thickness distribution can be directly estimated from the calculated flux distribution of sputtered particles to the substrate. Moreover, the velocity distribution function of sputtered particles reaching the substrate is also obtained, and it can be expected to be associated with the evaluation of the film quality and the evaluation of the embedding characteristics in fine trenches.

Simulation technologies such as heat, fluid, structure, electromagnetic waves, etc. have already been widely used in the design of buildings, automobiles, aircraft, electronic equipment, etc., and have succeeded in greatly reducing the experimental and prototype cost.

Also, in this field, many easy-to-use commercial software is sold, contributing to the spread of simulation technology. Research on plasma simulation has also been widely conducted by many researchers and has made great use in understanding of plasma phenomena. However, it is true that technicians have not yet accepted widely as a design tool of the device. The reason is that calculation load is large, lack of cross sectional data, chemical reactions occurring on the surface are not well understood, measurement data in the apparatus is hardly available, evaluation of accuracy of calculation results is difficult, etc. For at least the maintenance of atomic and molecular data, a unique organization in Japan will be necessary.

Conclusion

In an r.f.-d.c. coupled magnetron sputtering system, the magnetron discharge was generated by a 13.56 MHz r.f. source, and a d.c. power was simultaneously applied to a tin target through a low-pass filter in order to control the incident ion energy on the target. When an extremely low r.f. power 5W and d.c. power sources were applied simultaneously to the target, the glow discharge was about one-seventh of that in the case of the d.c. magnetron discharge.

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