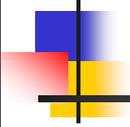
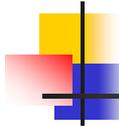


Evaluation of the Cu atomic density during sputter deposition process with optical emission spectroscopy



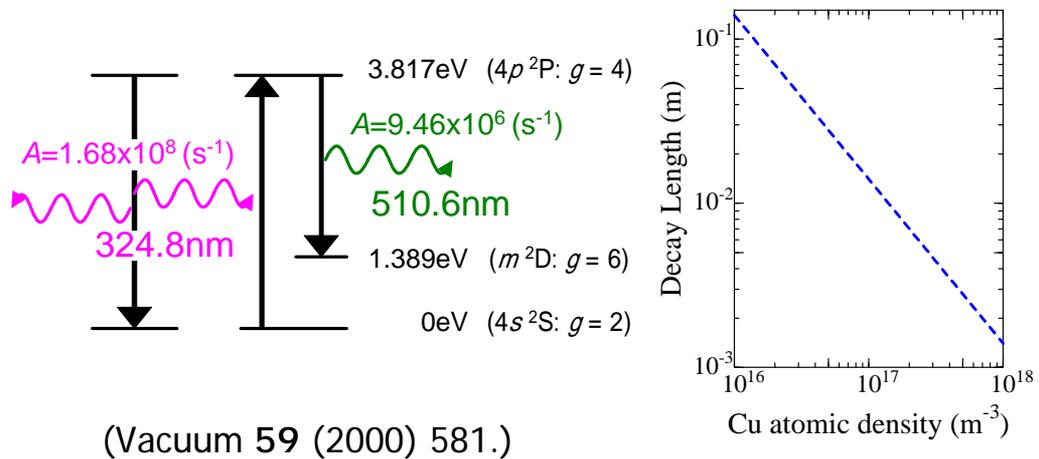
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Outline

- Optical Emissions and absorptions between low-energy levels of Cu neutral
- Evaluation of copper atomic density using intensity profiles of 2 emission lines from CuI
- Comparison with the atomic density deduced from a one-particle Monte-Carlo simulation

Energy levels of Cu neutral



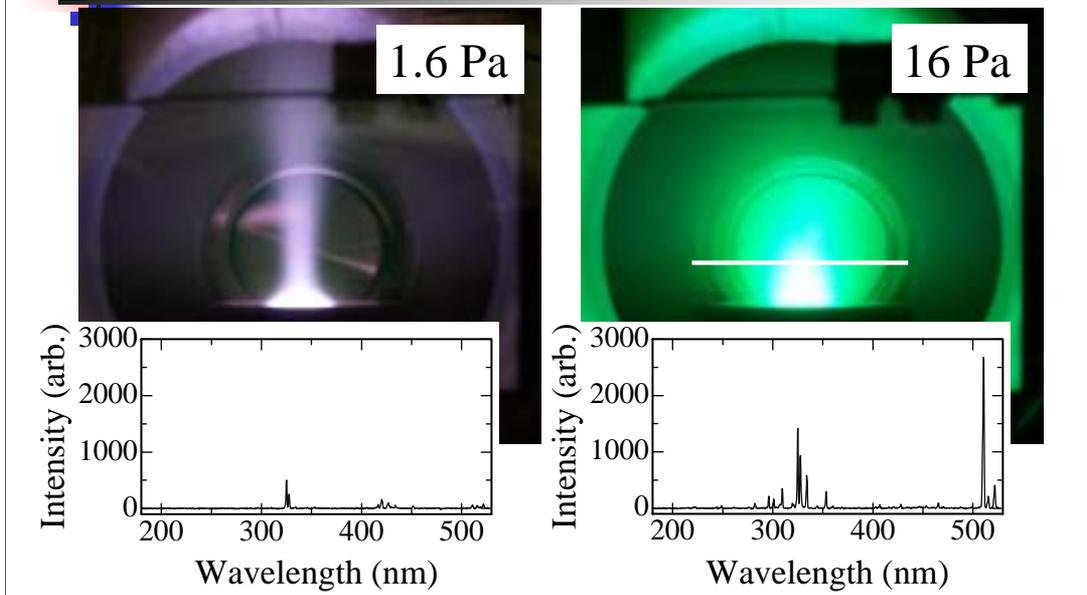
In this viewgraph, energy levels used in this study are shown. The line at 0eV is the ground state of Cu, and there is an excited state at 3.8 eV above the ground state. The transition from this state to the ground state is permitted, and 324.8 nm emission occurs. There is another transition from this state to the intermediate state, which causes 510.6 nm emission.

The transition probabilities of these emissions are also shown. The probability of 324 is about 20 times larger, so this emission occurs more preferably.

We have been observed these two emissions from the copper sputter plasma, and found that the 510 emission becomes relatively stronger when Cu atomic density is high. For example, high discharge power or high gas pressure cases. We think that this is due to the absorption of 324 emission by other copper atoms at ground state in the plasma environment. This self-absorption effect is well known to chemists using plasma emission for their quantitative analysis.

The right part of this viewgraph is the relation between the decay length of 324 emission and Cu atomic density. Both axes are in log scale. Decay length is about 1 centimeters when atomic density is 10^{17} per cubic meters, and is inversely proportional to the atomic density.

Sputter Plasma



These are the photographs of the sputter plasma we observed. The left is at 1.6 Pa, and the right is 16 Pa. You can see remarkable green emission at higher gas pressure case. The emission spectra of these plasma are given at the bottom. They are taken at about 1cm above the target.

At 1.6 Pa, 324 emission can be seen clearly, and 510 emission is weak. It reflects the difference of transition probabilities of these spontaneous emissions. The purple color of the discharge is derived from Argon lines around 400~450 nm.

At 16 Pa, we can still see the strong 324 emission, but 510 emission is also very strong. This relative increase of the 510 emission is caused by the absorption of 324 emission.

OES measurement

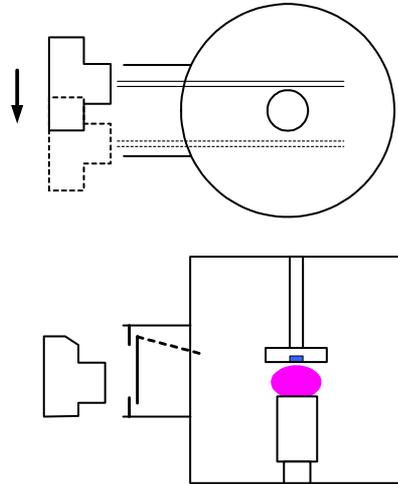


We observed the optical emission from the plasma with an equipment shown in this photograph. There is a quartz viewport of 7 times 5 centimeters, and the sputter chamber is located at the right side of this photo.

The camera body at the left is a commercially available reflex camera, but the lens is replaced with a quartz plano-convex lens, and the intake of this optical fiber is placed at the focal point of the lens. The optical system is mounted on this PC-controlled stage and moves horizontally.

OES measurement

- Optical System with an iris (2.0mm ϕ) and a plano-convex lens
- Wavelength 185 ~ 525nm (with 1024 channels)
- Balanced-magnetron (target 5cm)
- DC power 50 W
- Ar flow-rate 10 sccm
- Ar pressure 1.6 ~ 16 Pa



This is a schematic drawing of the measurement. The modified camera moves automatically as shown in the top view.

With an iris and the plano-convex lens, we can collect the emission from the tube region. And by sweeping the camera, we obtain the emission profile of the plasma.

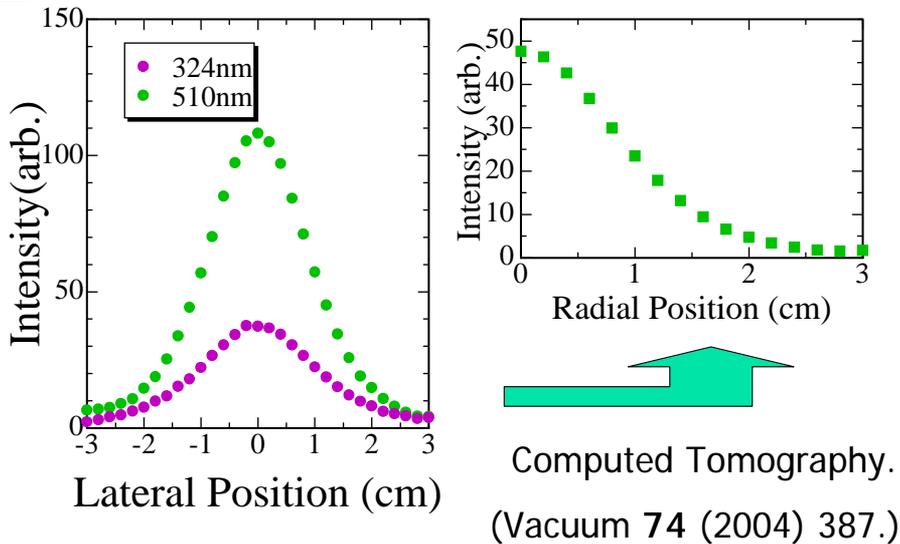
The collected emission is lead to the spectrometer by the optical fiber, and the spectrum between 185 and 525 nanometers is recorded with an CCD array of 1024 channels.

The sputter plasma was generated by the balanced type magnetron HERE. Cu target is a disc form and its diameter is 5 centimeters. It is located at the symmetric axis of the chamber, so we can expect that the plasma is also axisymmetric.

DC power was 50 watts in this study. Argon flow rate was 10 sccm, and the pressure is changed from 1.6 to 16 pascals.

It was not appeared in the previous photos of plasma, but in actual measurements, substrate holder was located at 4cm above the target. At the center of the holder, thickness monitor is equipped and the deposition rate of copper film was recorded during the OES measurement.

Emission Profile (16Pa)



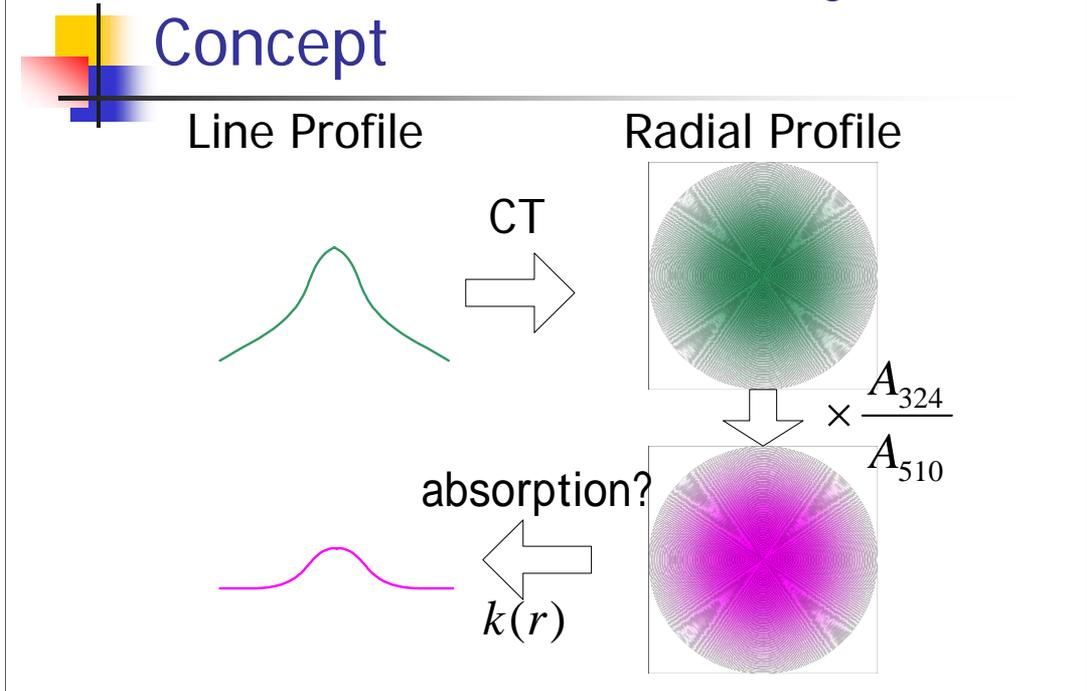
This is an example of the emission profile of 324 and 510 emissions at 16 Pa. It is taken at 1 cm above the target, and the camera was moved parallel to the target surface. At this pressure, 510 emission is stronger than the 324.

In case of no absorption, we can apply a computed tomography technique to obtain the radial emission profile. Please note that the system is axisymmetric. So the line profile from 1 direction is OK to reconstruct the profile. By applying the CT to 510 emission, we can obtain the radial profile like this.

We can expect 324 emission also has the form like this, with the ratio of transition probabilities. However, it is absorbed as it passes through the sputter plasma region, the observed intensity profile becomes weak.

Evaluation of Cu density:

Concept



In this cartoon, I would like to explain the concept of the density evaluation.

By the OES measurement, we can obtain the side view line profile of 324 and 510 emissions like the ones at the left. Because our chamber is axisymmetric, we can construct a radial profile by Computed Tomography, if the absorption can be neglected. And we neglect the 510 absorption, and calculate the radial profile.

When the spontaneous emission is dominant, the ratio of the emission profile of 324 can be determined from the 510 profile and the ratio of transition probabilities of both emission. Actually, the transmission function of the measurement system is also taken into account.

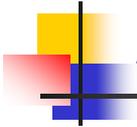
If there is no absorption for 324 also, the side-view line profile is obtained by the line integral of this radial profile and have the profile 20 times larger than the 510 profile. But it is not the case in actual measurements, so we have to consider the distribution of absorption coefficient. It should be axisymmetric, too.

And from the absorption coefficient, we can evaluate the atomic density of Cu at ground state.

In summary, I can say that we are making the absorption measurement using the plasma itself as a light source.

Evaluation of Cu density:

Assumptions



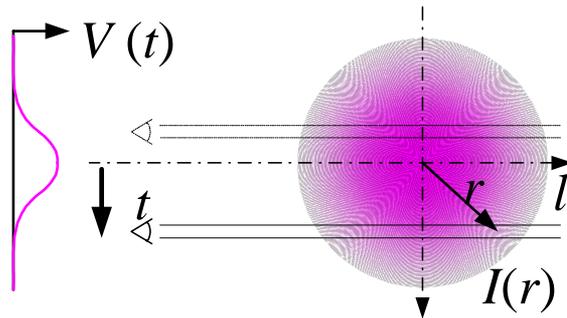
- Radial emission profile of the 510.6 nm line can be obtained by the Computed Tomography (no absorption for 510.6 nm).
- Emission profile $I_{324}(r)$ of 324.8 nm line is given by the 510.6 profile and the ratio of transition probabilities of these emissions.
- Absorption coefficient $k(r)$ for the 324.8 nm line is determined by the density of Cu atoms at ground states.

This slide summarize the assumptions of this method. Actually, we have to say they may be quite naïve in some cases.

Evaluation of Cu density: Effect of the Absorption

$$V(t) = \int dl I_{324}(r) \exp\left\{-\int_{-\infty}^l dl' k(r')\right\}$$

$$r^2 = t^2 + l^2, \quad r'^2 = t^2 + l'^2$$



The relation between the radial emission profile, absorption profile, and the side-view line profile is shown in this viewgraph.

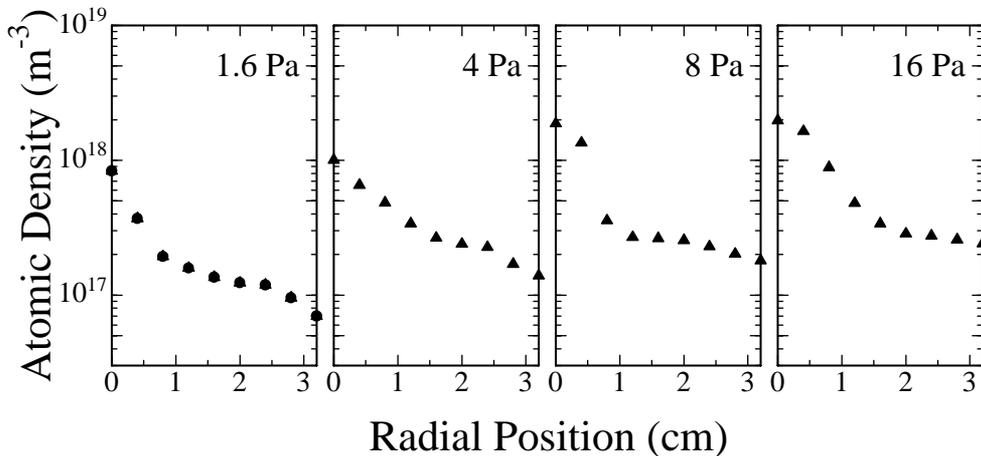
This is a plane by which the plasma is cut parallel to the target face, and here we place an origin on the symmetric axis.

t axis denotes the direction along which the camera moves and takes the line profile. And l axis is perpendicular to the t axis. Radial distance r from the center is given by these two coordinates.

The line profile V has a form of integration. The contribution at l dl is, the emission there, times the exponential of the integration of the absorption coefficient.

In this case, V and I are known, we should be able to determine $k(r)$ by solving this inverse problem.

Radial profile of the Cu atomic density

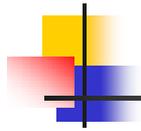


Unfortunately, at the moment, we have not found an analytical solution of this inverse problem. So we tried to represent the absorption profile by a spline function. And by moving the nodes to reproduce the side-view line profile as well as possible, we obtained these atomic density profiles.

Actually, if we move every nodes freely, the noise of higher frequency component appears and some of the results show unreasonable oscillations. So we have to add one more limitation that the density profile is a decreasing function with r , that is, a node cannot be larger than the inside neighbor.

The resultant density was the order of 10^{17} to some 10^{18} m^{-3} , and generally increased as the argon gas pressure increased.

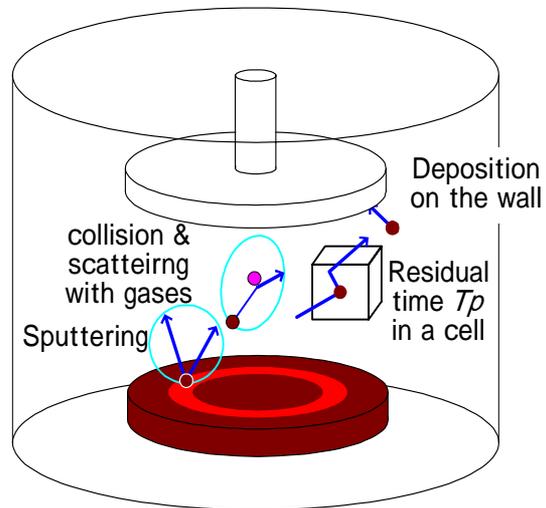
The order of the density corresponds to the decay length of some centimeters to millimeters. It is the similar order with the size of our sputter system, and that's why the ratio of the intensity changed significantly in our case.



One-particle MC Simulation

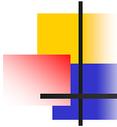
Monte Carlo simulation of the sputtered particles treats the “life” of them through:

1. Sputtering ejection from the target.
2. Collision and scattering with gas atoms
3. Deposition on the chamber wall.



From now on, I'd like to talk about another approach to evaluate the atomic density using one-particle Monte Carlo simulation.

This is a method to chase sputtered particles one by one from they sputtered from the target, collides and scattered by the ambient gas atoms until they reach some part of the chamber wall. With trials of some millions of particles, we can obtain the distribution of arrival flux on the substrate as well as chamber boundary.



One-particle MC simulation (2)

(Appl. Surf. Sci. 113/114 (1997) 642.)

- **Boundary Condition**
 - Axisymmetric
 - Uniform gas temperature (400K) and pressure
 - Sticking Coefficient at the boundary is unity.
- **Ejection of the particles**
 - Position proportional to the erosion track depth
 - Energy Thompson's formula
 - Angle cosine law
- **Scattering with gas atoms**
 - Thermal motion of gas atom (Maxwellian)
 - Elastic scattering with the Born-Mayer potential
($U(r) = A \exp(-br)$)

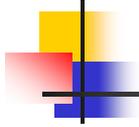
The detail of the MC simulation we used is summarized here.

We use an axisymmetric boundary, uniform gas temperature at 400K and uniform gas pressure. Sticking coefficient at the boundary is assumed to be unity.

Ejection of particles is proportional to the erosion track depth measured after the actual sputtering experiment, ejection energy distribution is Thompson's formula, and angular distribution is the cosine law.

This simulation includes the thermal motion of colliding gas atoms as Maxwellian. Scattering process is assumed to be elastic, and we used the Born-Mayer type repulsive potential.

Density evaluation by the MC simulation



- Split the space into cells
- Count the staying time T_p of Cu atoms in each cell during the simulation
- Compare the arrival flux of atoms (simulation) with the experimental deposition rate, and obtain T_s
- Average atomic number in each cell is given by T_p / T_s

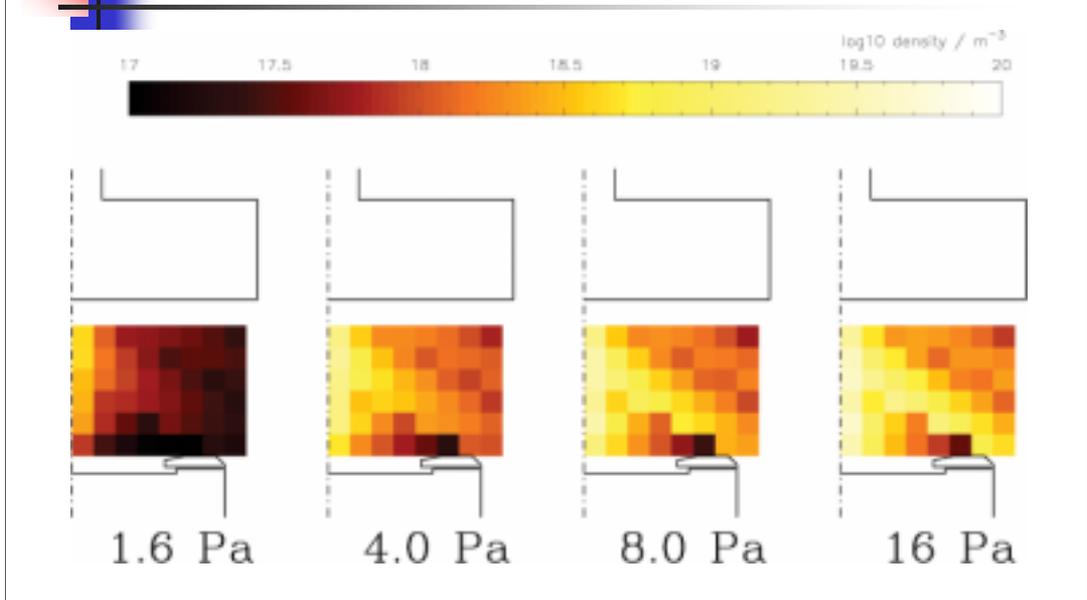
Using this one-particle MC simulation, we deduced the atomic density as follows.

Before the simulation, we split the chamber space into cells, and we count and sum up the staying time of trial atoms T_p during the simulation.

At the same time, we compare the arrival flux of atoms by the simulation, with the actual deposition rate at the same place of the chamber. By this, we can elucidate the time T_s of the simulation corresponding to the actual deposition experiment.

And by dividing T_p by T_s , we can obtain the average number of atoms in each cell, and we can obtain the density from the cell volume.

Atomic density profile of Cu (MC calculation)

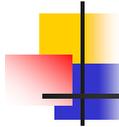


And this is the result of the simulation. Target face is here, and this is the substrate holder. At the center of it, there is a thickness monitor. The deposition rate in this case was about 0.8 nm/s at 16 Pa, and 1.5 nm/s at 1.6 Pa.

The color bar is given at the top in log scale, from 10^{17} ~ 10^{20} m⁻³.

The position we made the density evaluation by OES is 1 cm above the target so around here. The value is about 10^{17} ~ 10^{19} , similar to the OES values.

You can also see that the higher argon gas pressure is, the higher the Cu atomic density is. It is also the same tendency with the OES result.



Summary

- A method is proposed to evaluate the atomic density profile of copper sputter plasma using the Optical Emission Spectroscopy.
- The result was agreed with the one obtained by the one-particle MC simulation in:
 - $10^{17} \sim 10^{18} \text{ m}^{-3}$ of density was obtained.
 - The higher the pressure was, the higher the atomic density became.
- The solver of the inverse problem should be improved.

<http://surf.ap.seikei.ac.jp/~nakano/>