Crystal Orientation Control of Au Thin films in Ion Beam Deposition Processes

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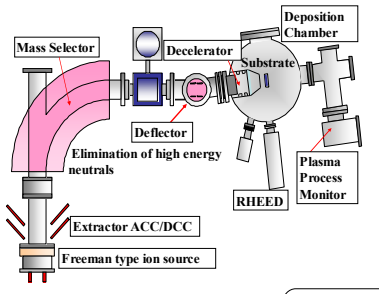
I. Introduction

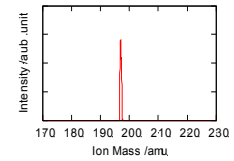
Thin metal film deposition techniques with various processing plasmas have been studied for fabrication of integrated circuits. In general, properties of deposited metal films are strongly influenced by the plasma parameters and substrate characteristics, such as ion and electron energies, plasma densities, and lattice constants. Among these, one of the most important factors affecting deposited metal thin film properties is considered to be the ion energy. **The ion energy effects on crystalline growth** have not been fully understood to date.

In this study, we have deposited Au thin films using a **low energy mass selected ion beam system** in order to investigate **the ion energy dependence of crystalline orientation** of deposited films. **Au** was chosen as the target material because of its inertness, which allows us to avoid additional effects of oxide or nitride formation due to residual gases in the system. The film structures were examined by **RHEED**, **XRD** and **AFM** analyses.

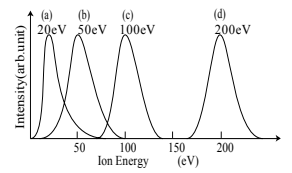
II. Experimental Setup

Extremely Low Energy Ion-beam Deposition System





Mass spectroscopy of ion beams



Energy distributions of Au+ ion beam

Experimental condition for Au film deposition	
Ion energy	20 – 200eV
Substrate	Untreated Si(100)
Environment	Less than 10^{-5} Pa
Temperature	Room Temperature
Averaged current	0.50 – 0.65 μA
Irradiation time	280 – 350 min.
Estimated film thickness	14 – 20 nm

Features of the system

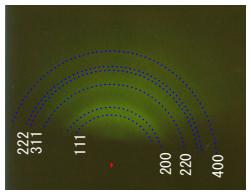
- High selectivity of ion species by mass selector
- Generation of Au ions in Freeman type ion source by sputtering
- Energy deviations were about ±10eV
- Untreated Si(100) substrate minimize the effect of lattice misfit.

Investigation of Au film formation processes by low energy ions is possible

III. Results

The crystalline structures and surface profiles of deposited Au films were examined by Reflection High Energy Electron Diffraction (**RHEED**), X-Ray Diffraction (**XRD**) and Atomic Force Microscopy (**AFM**).

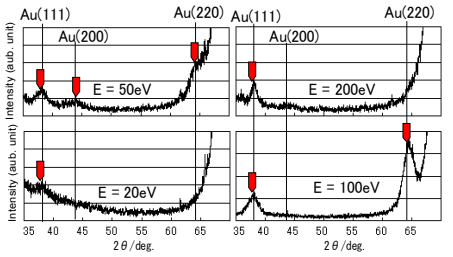
3.1 RHEED



RHEED pattern of Au film deposited at 55eV

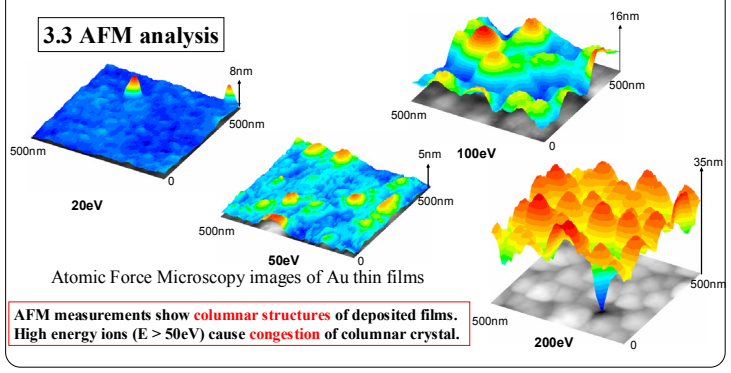
Polycrystalline Au films are deposited on the untreated Si(100) wafer.

3.2 XRD Analysis



The dependence of crystalline orientation on the incident ion energy is clearly seen.
- **The peak of a Au(111) plane is visible for all injection energies.**
- **The presence of Au(220) planes is shown at 50eV and 100eV.**
- **The Au (200) peak at 100eV is remarkably large.**

3.3 AFM analysis



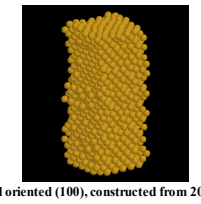
Atomic Force Microscopy images of Au thin films

AFM measurements show columnar structures of deposited films. High energy ions (E > 50eV) cause congestion of columnar crystal.

IV. Molecular Dynamics Simulation

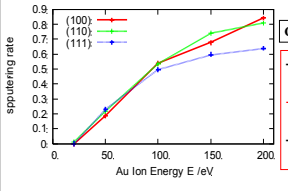
Molecular dynamics simulation using a glue model was carried out for determination of the mechanism of preferred orientation in low energy ion beam deposition.

- **Number of Injection : 1,000 times**
- **Simulation period : 2ps**
- **Temperature : 300K**
- **Ion Energy : 20 – 200eV**
- **Applying a periodic boundary condition for x and y direction**
- **Each simulation was performed independently.**



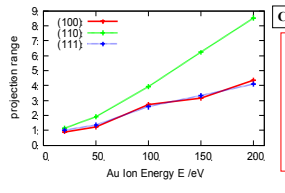
Substrate model oriented (100), constructed from 2016 atoms

Simulation results with glue model



Calculation of self sputtering rate in Au low index surfaces

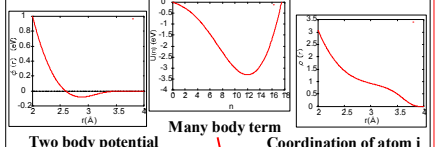
- **In lower energy range (E < 100eV), no difference is found among the three low index surfaces.**
- **In higher energy range (E > 150eV), Au(111) surface shows lower sputtering rate than other low index planes.**
- **Calculation results for the Au(100) and Au(111) surface present similar trend.**



Calculation of projection range of Au low index surfaces

- **Projection range of Au(111) and Au(100) are about the same value.**
- **Ions irradiated on Au(110) surface are easily penetrate.**
- **In higher energy range (E > 150eV), Au(111) surface shows lower sputtering rate than other low index planes. It seems that the higher surface free energy decreases desorption.**

Glue Model



$$V = \frac{1}{2}\sum_{\substack{i,j=1\\(j\neq i)}}^{N}\phi(r_{i,j}) + \sum_{i=1}^{N}U(n_i), \quad n_i = \sum_{i=1}^{N}\rho(r_{ij}),$$

$$\mathbf{F}_i = -\sum_{i\neq j}\left(\phi'(r_{ij}) + \left[U'(n_i) + U'(n_j)\right]\rho'(r_{ij})\right)\frac{\mathbf{r}_{ij}}{r_{ij}}.$$

- **Description of an empirical many body scheme named 'glue' model**
- **Good unified description of bulk, defect and surface properties of gold**
- **Reproducibility of Au surface reconstruction**

F. Ercolessi, M. Parrinello and E. Tosatti, Philosophical Magazine A, 1988, Vol. 58, No. 1, 213-226

Features of Au low index crystal surfaces

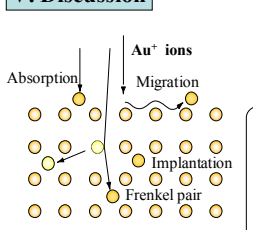
(100)
- **Activation by ion energy enhances crystal growth. (50eV)**
- **Self sputtering was caused in higher energy (100eV -)**

(110)
- **Activation by ion energy (50 – 100eV).**
- **The most open channel in Au decrease self-sputtering. (100eV -)**

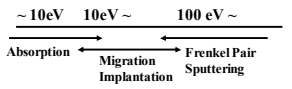
(111)
- **The higher surface energy of Au(111) results in lower sputtering rates.**
- **Preferred orientation in wide energy range.**

Possibility of controlling crystal structure by selecting adequate ion energy.

V. Discussion



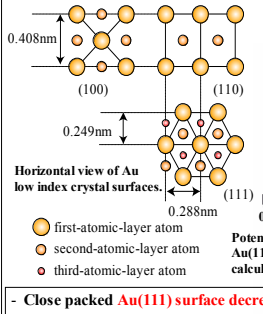
Processes in solids on ion impact



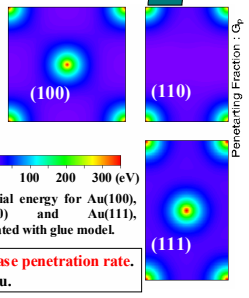
Ion Energy Effect

- Absorption in low energy range (~20eV)
  - **Stability of surface dominate the crystal growth.**
- Migration of adatoms and **enhancement of crystal growth** (10eV~)
  - Implantation cause **subsurface process**.
- **Damage** from generation of Frenkel pair and sputtering (100eV~)
  -Self sputtering is dominant.

The Difference of Ion Energy Effectivity for Penetration on Three Low Index Surfaces

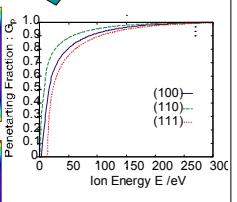


Horizontal view of Au low index crystal surfaces.



Potential energy for Au(100), Au(110) and Au(111), calculated with glue model.

Potential > Ion energy → Penetration



The energy dependence of penetrating fraction of each low index plane calculated with the glue model.

- **Close packed Au(111) surface decrease penetration rate.**
- **Au(110) has most open channel in Au.**

VI. Summary and Conclusion

Au thin-film deposition was carried out with the low-energy mass-selected ion-beam deposition method. The **ion-energy dependence of crystal structures** was investigated with XRD and AFM.

Molecular dynamics simulation was performed for determination of the **mechanism of preferred orientation in low energy ion beam deposition**.

- The experiments have shown that the **crystalline orientation can vary with the incident ion energy**.
- AFM measurements show **columnar structures** of deposited films.
- **The planes with relatively high surface energies were shown to be formed** due to the ion-energy effect.
- Activation and self sputtering caused by ion energy affects crystal growth.
- The possibility of **controlling the crystalline structure of the deposited films by selecting adequate ion energies** was pointed out.