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Simulation of silver thin films under different flux angles and influence of deposition rate on growth

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Abstract:
Among the transition metals, Silver is crucially important. As this metal has a high electrical and thermal conductivity, its thin films have been used for the internal connections of integrated circuits. Furthermore, its resistance against the metal electrical migration is more than aluminum. Conductivity in thin films has a significant correlation with the both grain size and texture of film. In this paper, researcher employed FACET software to measure the final grain size through deposition in the angle flux conditions. The angled flux condition of a facet can be shielded from the flux, such that it does not receive any deposition flux. In the first stage of experiment, the final grain size was measured under angle flux condition while the deposition rate was increased at a constant temperature. At the final stage, the final grain size was measured in different flux angles. The influence of deposition rate on final grain size is investigated under angle flux**.** We increase the deposition flux providing that temperature of substrate is fixed and in a low quantity**.** Computer simulations show that the final grain size was increased with increased deposition rate.

Key words: Simulation, Silver thin film, FACET, Angle flux

I. INTRODUCTION

Over the recent years the research in thin layers has been attracted by the researchers focusing on the implication of thin layers for using in industries such as producing electronic integrated circuits, magnetic and optical ambient for recording information, a decorative and protective covers, reflective and optically pass, layers, acoustic thin layers sun cues which are some amongst the others. In addition, producing thin layers of diamond and carbon nanostructures would be possible by the use of thin layers technology. Moreover, developing nanotechnology sciences and evolution which this science is creating in the industry and our life increased the scholars’ attention to the thin layers industry. In fact, the diversity in microstructure and nanostructure of thin layers has main role in its significant growth in recent years. For example, Layers with network structure are able to highly attract light as well as showing chemical reaction to their environment. This ability in thin layers would be the reason for using them light cells, gas heat sensors and/or catalistic environment.

Different characteristic of thin layers does depend on their micro- and nano-structures and studies being carried out in this area intend to:

-optimize different characteristic of thin layers,

-control and make the producing process replicable,

-to have better understanding of growth mechanism of thin layers and

-to discover new applications for thin layers

Heat evaporation is one of current methods to produce thin layers. Deposition conditions in some way affect characteristics of micro and nanostructure of thin layers such as forms, or the size of layers, constituent blocks or grains, the distribution function of the size of grain and preferential direction. These elements being synchronous makes the problem more complicated. Deposition conditions in each process with special mechanisms affect forming thin layers. In this paper forming and evaluating structures of thin layers would be considered by FACET software and how micro- and nano-structure parameters of thin layers are affected would be described.

II. SIMULATION AND THIN FILM

In the semiconductor industry, computer simulations would be extremely useful to be able to predict the profile and microstructure (grain size, grain shape, grain orientation, texture and roughness) of polycrystalline thin films as a function of their deposition conditions (temperature, flux distribution, deposition method, substrate geometry, materials). In general, computer simulations can reduce experimental costs and decrease overall development cycle time.

The idea of reducing the triple junctions and grain boundary pathways can be extended to the extreme by considering single crystal interconnects, which were observed to be nearly immune to electro migration damage F.M. D'Heurle et al. (1970).

In this work, we discuss a two-dimensional multi-scale model to simulate thin film growth, including deposition, nucleation, surface diffusion, grain growth and grain interaction. FACET fills the gap between atomic and feature scale models of thin film growth.

The diffusion rates determine and final texture of the film. FACET determines growth rate of each grain, and thus control the morphology.

Knowing the diffusion activation energies, it is possible to calculate the atomic flow rates between adjacent facets by a kinetic lattice Monte Carlo method. The results from a sophisticated three-dimensional KLMC calculation can be input to FACET, but because of the complexity of the full scale KLMC methods, only the rates for Cu atoms diffusing from {1 0 0} to {1 1 0} and {1 1 1} have been achieved in the previous Z. Wang (2000) .

At present, there is no good model for heterogeneous nucleation, so user can by FACET the nucleation rate, nuclei size, and texture are determined.

Many factors can affect the nucleation rate of islands, such as temperature, gas pressure, deposition rates, contamination, defects, etc. After nucleation is finished, FACET determines facet growth rates based on deposition and diffusion between the facets, and diffusion from the surface to the nuclei. At every simulation time step, FACET calculates the length of each facet, the number of atoms deposited on that facet, and the number of atoms diffusing to and from the facet to adjacent facets and surfaces. Then, it calculates the net change of atoms on each facet, and translates that into the growth rate.

III. FACET MODEL APPLICATION

Users have a wide degree of control of the simulation and visualization. It is important to note that FACET only directly simulates film growth, and not nucleation. FACET has been constructed to simulate, visualize and analyze polycrystalline thin film growth in two dimensions. The following are the parameters that can be tuned to different experimental conditions:

- Deposition rate
- Deposition time
- Substrate temperature
- Nuclei density
- Random or ordered placement of nuclei
- Nuclei texture: This is related to the materials

FACET allows any combination of {1 0 0} oriented, {1 1 0} oriented, {1 1 1} oriented, and random nuclei. For example, FACET can generate and grow a thin film within which 30% of the nuclei are {1 0 0} oriented, 50% are {1 1 0} oriented, and 20% are random oriented.

IV. FLUX CONDITIONS

FACET can simulate the following four types of flux conditions:

1. Direct deposition
2. Equal flux
3. Angled flux
4. Alternating flux

Allow the user to alternate the flux direction up to six times. Thus, there are a total of 10 factors that could be varied.

In order to design a model by logical simplifications to be able to show the most important physical processes, the following hypothesis are designed and provided:

1- This model is a 2D stimulator.
2- The grain boundary surfaces are drawn via line. Each surface is described via one line.
3- Each nucleus has its specific direction which affects facet growth rates.
4- Nuclei density, initial size and texture are input parameters.

This model is severely reducing calculation expenses and can perform easily on a PC. This model provides qualitative and semi-quantitative results for large systems Z.Wang et al. (2002).

A. Influence deposition rate on final grain size under angle flux

In this section, the influence of deposition rate on final grain size is investigated under angle flux. The angle flux condition a facet can be shielded from the flux, such that it does not receive any deposition flux. However, the shielded facet will still interact with the adjacent facet and contribute to the film microstructure evolution by inter-facet diffusion. The angle flux impacts the surface of substrate under angle of 45 degrees. We increase the deposition flux providing that temperature of substrate is fixed and in a low quantity. In this section of the tests, the output is final grain size based on thickness.

Figure 1 shown by increasing deposition rate the final grain size is increased. Figure 2 shown

Room temperature microstructure of typical simulated thin films with deposition rate of 10 Atom/nm.s under different flux angle of 10 degree (a), 40 degree (b), 60 degree(c).

B. The effect of flux angle on final grain size

In this part, the influence of flux angle on final grain size is investigation. This part of computerized experiment, while the deposition rate was fixed at a constant temperature, flux angle was varied. The flux hitting substrate surface in a certain angle is called angled flux. A surface can be shielded of flux in angle deposition, Hence, because many of facets remain shielded and the number of levels will be increased when the flux angle is increased, a very few number of atoms will remain under the flux angle. Figure 3 shows indicate the final grain size based on flux angle. According to this curve, by increasing flux angle the final grain size is increased.

CONCLUSION:

In the first stage of experiment, the influence of deposition rate on final grain size is investigated under angle flux**.** We increase the deposition flux providing that temperature of substrate is fixed and in a low quantity**.** Computer simulations show that the final grain size was increased with increased deposition rate.

At the final stage, experiment, while the deposition rate was fixed at a constant temperature, flux angle was varied. The angle flux condition a facet can be shielded from the flux, such that it does not receive any deposition flux. In angle flux conditions, because many of facets remain shielded and the number of levels will be increased when the flux angle is increased, a very few number of atoms will remain under the flux angle. Therefore, with more accumulation flux, the level of facets will find more opportunity to have surface diffusion. Resulting in creating more opportunities for the process of coalesce. In fact, the more increased surface diffusion, the bigger size of final grain.

Computer simulations show that the final grain size was increased under angle flux condition while the deposition rate was increased at a constant temperature. The final grain size was increased in different flux angles.

REFRENCES:

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Figure captions

Fig. 1 The final grain size via deposition flux in the flux angle Θ = 45.

Fig. 2 Room temperature microstructure of typical simulated thin films with deposition rate of 10 atom/nm.s under different flux angle of 10 degree (a), 40 degree (b), 60 degree(c).

Fig. 3 The final grain size via different flux angles in the temperature of T=298 K.

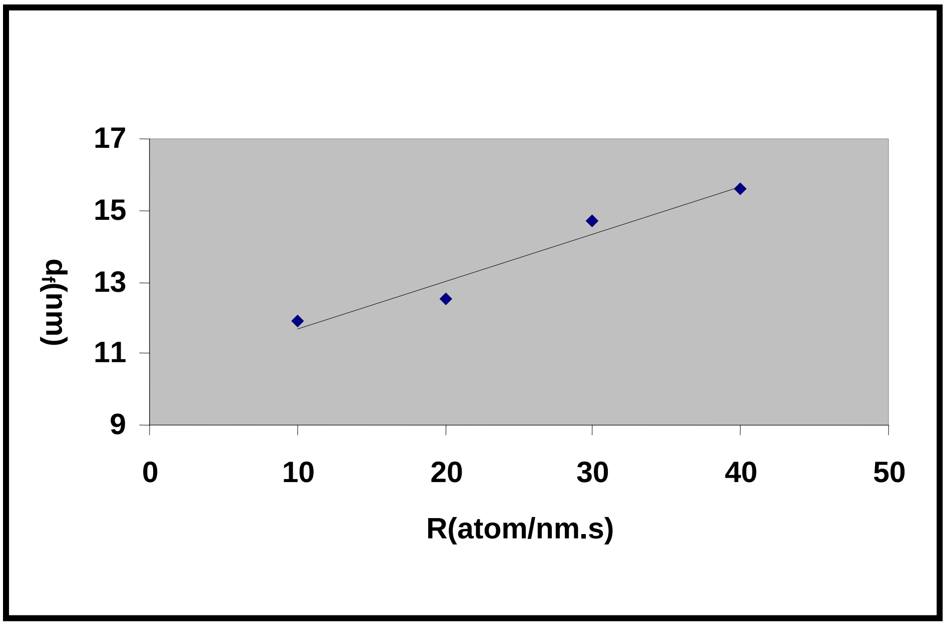
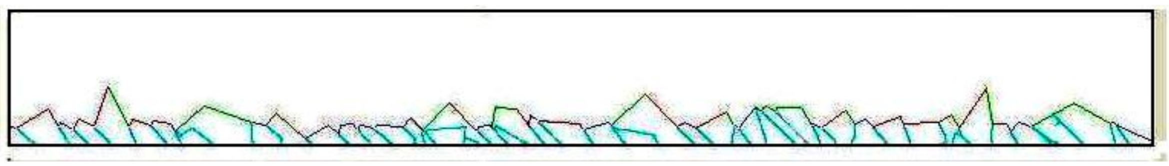
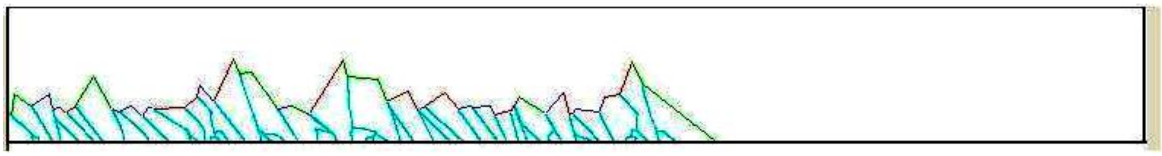


Fig. 1



(a)



(b)

Fig. 2

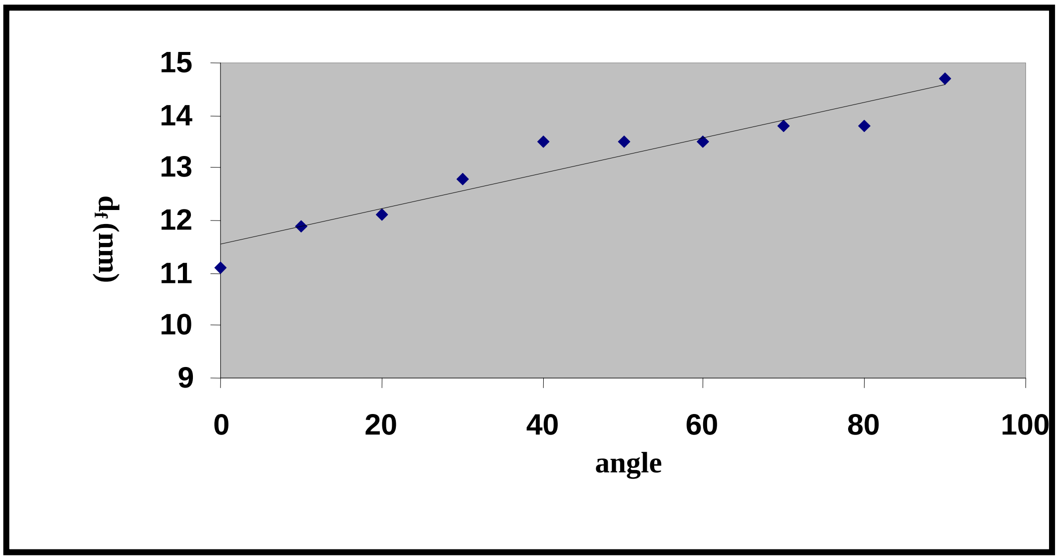


Fig. 3