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Filling the Submicron Contact Holes with Al Alloys

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Al 합금의 Contact Hole Filling에 관한 연구

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Abstract — Submicron contact hole filling with aluminum alloys has been achieved with a multi-step metallization method, which utilizes a metal "flow" or self-diffusion process at elevated temperatures after the metal was sputter-deposited. A multi-chamber, modular sputtering system was employed to deposit aluminum alloys and subsequently to anneal the deposited metal films under vacuum at high temperatures. The films were deposited on 200 mm wafers with planar, dc magnetron sputtering sources without any substrate bias. The basic process steps studied for the multi-step metallization include an initial layer deposition at low temperatures, less than 100℃, and an annealing step at elevated temperatures, between 450 and 550℃. The degree of planarization or step coverage was dependent strongly upon the temperature and time of the flow step and complete filling of the submicron contacts with aluminum alloys was achieved. Responsible mechanisms for the enhancement in step coverage and factors determining uniform and reproducible flow of aluminum alloys during the high temperature step are discussed.

요　약 — 진공 증착 혹은 증착 후 Al 박막을 고온에서 열처리하여 submicron size의 contact hole에 Al 막을 메꿀 수 있는 공정 및 그 역학(mechanism)에 관하여 연구하였다. Multi-chamber 스퍼터링 장치를 이용하여 Al막의 증착 및 웨이퍼의 이동, 그리고 다음 chamber들에서의 열처리 등 모든 과정이 진공하에서 이루어졌고, 박막의 스퍼터링은 200 mm 웨이퍼상에 dc magnetron source를 사용하여 bias 없이 증착되었다. 공정순서는 처음 단계에서 저온 즉 100℃ 이하에서 Al을 증착시킨 후 450~550°C 사이의 고온에서 Al 막을 가열하여 Al이 contact hole에 fill이 되도록 유도하였다. Al 움직임의 주된 mechanism은 Al의 표면자기확산(surface self-diffusion)으로 고려되었다. 따라서 step converge의 향상 정도 혹은 Al의 평탄화 정도는 고온 공정의 시간 및 온도에 크게 좌우되었다. 또한 공정 결과의 재현성은 웨이퍼 표면의 청정도 및 온도 균일도가 주된 영향을 주는 요인임이 고찰되었다.

1. Introduction

Multi-step sputtering processes, which utilize an initial, cold deposited layer followed by a high temperature step, have shown very promising results on Al step coverage [1, 2]. Park *et al.* [2] reported that contact planarization in ULSI multi-level interconnections had been achieved by utilizing a high temperature post-heating between aluminum alloy depositions. Submicron contacts with an aspect ratio greater than 1 were completely filled by heating above 500℃. A full CMOS device [2] farbricated with this aluminum planarization method showed no degradation of electrical characteristics such as contact resistance and junction leakage due to the use of such high temperatures. In addition, reliability tests with line test patterns revealed better elctromigration resistance and stress migration tolerance than those using the conventional one-step deposited aluminum alloy lines.

As integrated circuit technology advances to lower submicron limits, achieving adequate step coverage in contact and via holes during the metallization processes become increasingly more challenging. The conventional "one-step" sputtering processes have been less than satisfactory in achieving adequate step coverage for submicron contact holes and vias. Since reliability issues in advanced circuits are primarily associated with metallization interconnect structures, it is quite important to establish a high performance, high reliability metallization scheme. Sputter deposition has been the most suitable process for metallization for many reasons and has been widely used for the current metal interconnect technology. Sputtering, however, has the inherent limitation on wall step coverage due to the directional flux of sputtered materials. As the contact and via dimensions become smaller, this limitation is even more critical because of "self-shadowing", which reduces the material flux at the bottom of the structure as well as on the side walls. In order to overcome such limitations and to fill contacts and vias, many techniques have been tried such as utilizing bias during sputtering [3-5], excimer laser application after metal sputter deposition [6, 7], and employing an elevated temperature during sputtering [8].

In the present paper, the methodology and mechanisms involved in the multi-step metallization process for filling the contact/via holes are discussed. Issues in utilizing the multi-step, high temperature process and directions for future developments are also discussed.

2. Experimental and Results

A multi-chamber, vacuum isolated sputtering system (Varian M2000/8) was employed for the experiments, as shown in Fig. 1. Each module of the system has its own cryo or turbo pump and is separated by an isolation valve between modules, allowing a true vacuum isolation during processing. Base pressures of the process modules were normally less than 3×10^{-8} torr during the experiments. Sputtering was performed with the Varian Quantum^{TM} source, which is a dc magnetron type with planar target. Each process module is equipped with a heater table capable of operation at 550℃ using a back-side argon gas heating system.

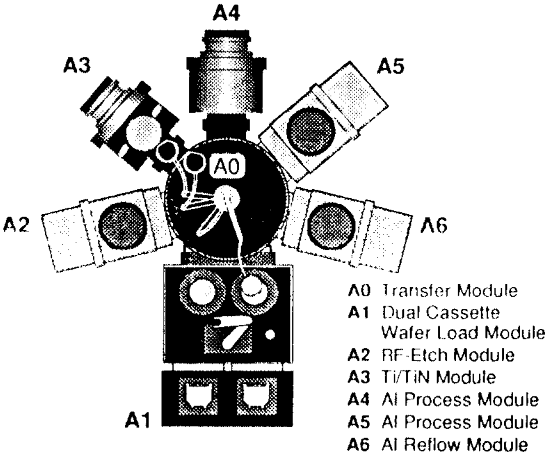


Fig. 1. Schematic of a multi-chamber, vacuum isolated sputtering system (Varian M2000/8) utilized for the experiments.

Fig. 2 represents SEM images of approximately 350 Å of Al/1%Si alloys deposited at 450℃ on two different substrates. The surface morphology shown in Fig. 2(a) was obtained from deposition on a 5000 Å layer of SiO_2 on a Si wafer and Fig. 2(b) was obtained from the alloy deposited on a 3000 Å layer of pre-deposited Al/Si.

The step coverage of a sputtered Al/1%Si/0.5%Cu alloy was evaluated over contacts of 0.8 μm diameter opened in a 1.0 μm thick thermal oxide on 200 mm wafers. In most cases before the deposition of Al alloys, layers of 300 Å of Ti and 1000 Å of TiN were deposited sequentially to provide a diffusion barrier, and the films were annealed in nitrogen for 30 minutes at 450℃.

Table 1 shows a list of various multi-step aluminum metallization processes. Among them, data from two experiments are compared in the present paper. Fig. 3 represents the SEM images obtained from an experiment in which a low temperature deposition was followed by a slow deposition at high temperature (Expt. A; Cold Dep + High Temp Dep in Table 1). The initial layer was a 0.35 μm thick,

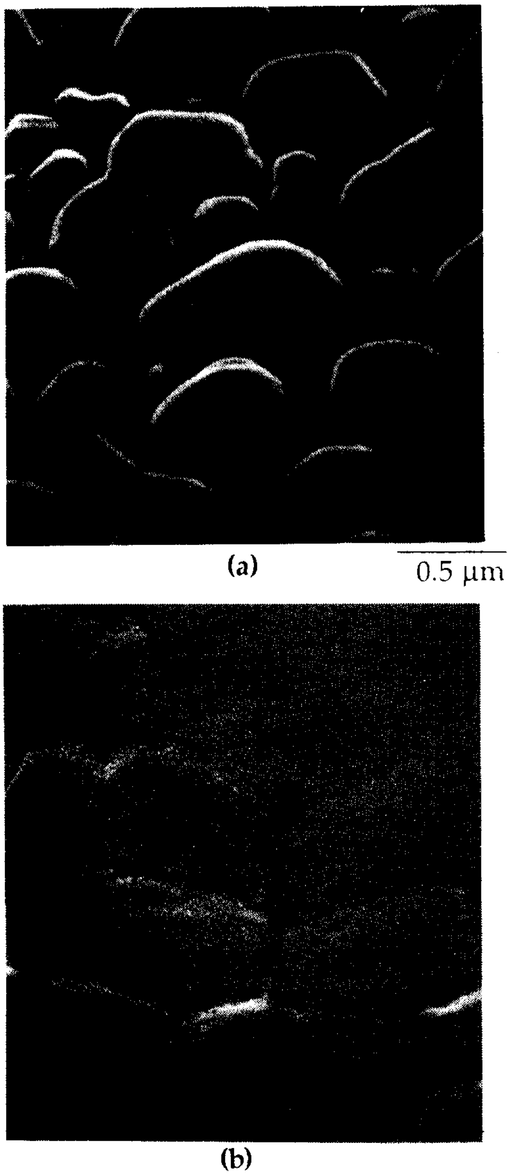


Fig. 2. Nucleation of 350 Å Al/1%Si deposited at 450°C on a SiO_2 layer (a) and on a 3000 Å Al/1%Si layer (b).

Al alloy deposited at 90°C. Following the initial layer, 0.55 µm of the Al alloy was deposited at 450°C. During the deposition, the total sputtering pressure was controlled at 2 mT. Fig. 3(a) shows the step coverage of a 0.8 µm contact, which has been filled with Al/1%Si/0.5%Cu to planarity. Bias was not applied during the process. The surface morphology of the film is shown in Fig. 3(b).

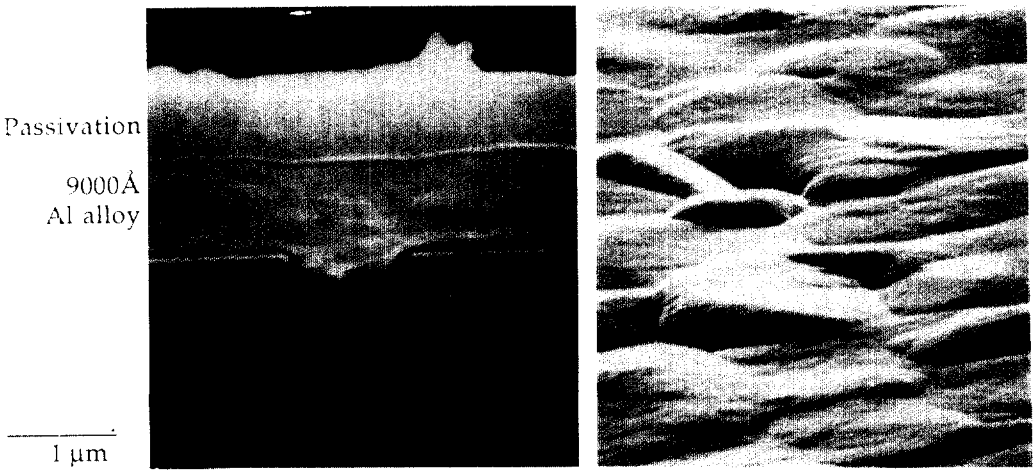
Fig. 4(a) presents SEM cross-sectional images obtained from an experiement using a low temperature deposition in the first module, a high temperature annealing without deposition in the second module, and finally, an additional low temperature deposition of the alloy in the third module (Expt. D; Dep + Flow + Dep in Table 1). The second step of annealing the deposited alloy at a high temperature involves a reflow of the deposited Al alloy without a vacuum break. In this case, the initial, 0.4 µ thick layer of an aluminum alloy was deposited at room temperature. The wafer was then immediately transferred to the second vacuum module and heated at 540°C for 180 seconds. After the flow, an additional 0.4 µ of aluminum alloy was sputtered at room temperature. Fig. 4(a) illustrates a 0.8 µm contact filled using this process. Fig. 4(b) shows the surface morphology of the film deposited by the dep-flow-dep process, which resulted in a smoother and higher reflectivity surface of the aluminum alloy compared to the two-step deposition of low and high temperature depositions shown in Fig. 3(b).

3. Discussion

Using a conventional one-step sputtering method at a low temperature, the achievable step coverage is limited due to low angle flux of sputtered materials as the feature sizes evolves to smaller than

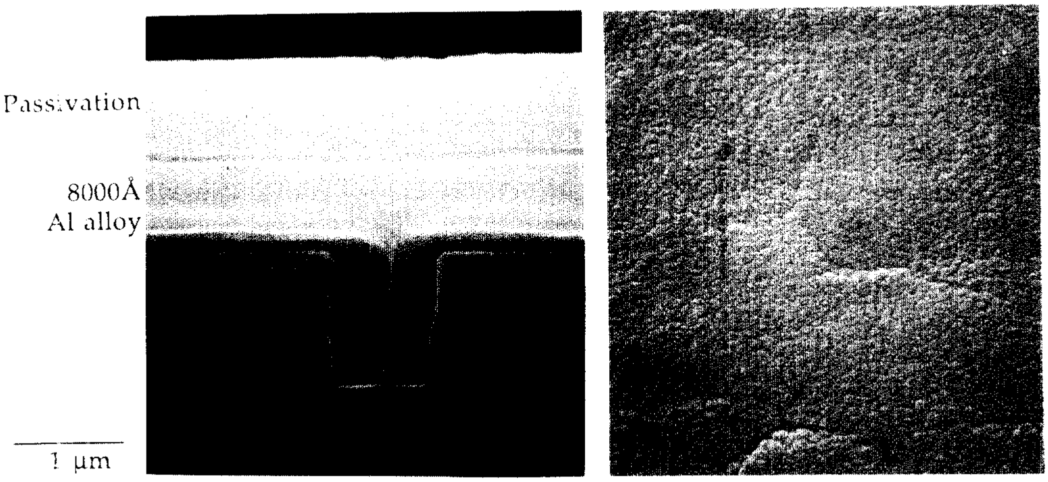
Table 1. Variations of the multi-step aluminum alloy metallization processes

	First step	Second step	Third step	Fourth step
Expt. A	Cold Dep.	+ High Temp. Dep.		
Expt. B	Cold Dep.	+ High Temp. Dep.	+ Cold Dep.	
Expt. C	Cold Dep.	+ High Temp. "Flow" (Without Dep.)		
Expt. D	Cold Dep.	+ High Temp. Flow	+ Cold Dep.	
Expt. E	Cold Dep.	+ High Temp. Flow	+ Cooling	+ Cold Dep.



(a) (b)

Fig. 3. SEM cross-section image of a planarized Al/1%Si/0.5%Cu film deposited an initial 3500 Å deposited at 90°C and followed by 5500 Å deposited at 450°C (a) and its surface morphology (b).



(a) (b)

Fig. 4. SEM cross-section image of a planarized Al alloy film using an inital 0.4 µm ambient temperature deposition followed by a 180 sec, 540°C reflow, and additional 0.4 µm deposition at ambient temperature for a total 8000 film thickness (a), and its surface morphology (b).

1 µm dimensions. The use of elevated temperatures during sputtering does increase the step coverage, but often results in voided films on the side wall or at the bottom of the submicron holes, due to the effects of surface tension. At elevated temperatures, the diffusivity of atoms is large so that atoms can travel long distances to find lower energy sites. When the surface energy of the substrate is lower than the vector sum of the energies of the Al alloy surface and the metal/substrate interface, the nuclei tend not to coalesce with each other to form a continuous layer. In such cases, the formation of a continuous film will require much thicker films (see Fig. 2(a)). Since materials deposited onto side walls and at the bottom of vias or contact holes are less than the other areas of the wafer surface during sputtering, the formation of voids or discontinuities in the film is more likely to occur on the side walls

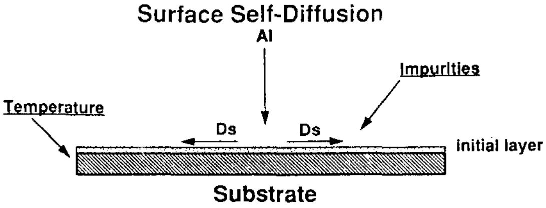


Fig. 5. Diffusion of aluminum alloys during the high temperature flow process. The impurity adsorption to the substrate surface and the substrate temperature uniformity are the most important factors in achieving the uniform flow.

and the bottom of holes.

3.1. Initial Layer Deposition at a Low Temperature

In order to eliminate such a voiding problem, it is necessary to have an initial layer deposited at a lower temperature, below 100℃. With the low mobility of atoms at a low temperature, a fine-grained, uniform film can be deposited on the substrate. The thickness required to keep the initial, fine-grained layer continuous during the following high temperature step is determined by the aspect ratio of the holes and the deposition temperature.

3.2. Surface Self-Diffusion at High Temperature

The next step in the multi-step process employs a high temperature in order to induce the "flow" of aluminum alloys, mainly by surface self-diffusion. This high temperature step can be done during aluminum alloy sputtering with a low deposition rate (Fig. 3) or by flowing the deposited alloy without any deposition (Fig. 4). It is, however, important to point out that the time between the initial cold deposition and the high temperature step should be minimized in order to reduce impurity adsorption to the surface of the initial layer. One of the underlying mechanisms involved in this process is the need to sputter aluminum atoms during the high temperature step onto the clean surface of the initial aluminum layer, so that aluminum can continue to grow without agglomeration during the high temperature step. Any vacuum breaks or high level of impurities, due to outgassing from the wafer or the process chamber, readily contaminates the surface of aluminum. This impurity contamination or reaction at the surface poisons the surface self-diffusion process of atoms and prevents the flow of aluminum for the planarization. One may not observe aluminum planarization by annealing the aluminum layer in a furnace once the wafer was exposed to air, because of an oxide layer formed at the surface. All processes during multi-step metallization for enhanced step coverage should be carried out under vacuum without vacuum breaks between steps, which is one of the main advantages in using the multi-chamber, vacuum isolated sputtering system. Since the diffusivity is exponentially dependent upon temperature, the uniformity of the "flow" over the substrate surface is likely to be determined by temperature uniformity. The precise control of wafer temperature and its uniformity, therefore, would be one of the key factors in achieving repeatable process results. During the sputtering process, however, the temperature uniformity of the substrate results from the combined effects of heat of condensation, ion bombardment, radiation and direct substrate heating. Thus, the wafer temperature uniformity is expected to be better during the high temperature annealing of the deposited alloy without deposition (Expt. D in Table 1) than it would be during a high temperature deposition (Expts. A and B in Table 1).

3.3. Additional Aluminum Alloy Deposition After the Flow Step

During the dep-flow-dep process, the additional deposition of aluminum alloy after the high temperature step provides additional flux for the aluminum flow until the wafer cools down and an ability to control the final film reflectivity. This step is performed at a low temperature and can be used to control the amount of silicon precipitates in the film when Si-containing Al alloys are used.

One of the main issues in the multi-step deposition process arises from the use of a high temperature step, which results in large grain size, low reflectivity, and deep grain boundary grooving on aluminum alloy films. The large grain size would be beneficial for better electromigration resistance.

However, alignment processes over the metal film are difficult because of the film roughness and the grain boundary grooves. For Al/Si alloys, silicon segregates to grain boundaries and layer interfaces during cooling from the high temperature step. Large Si precipitates are found along the grain boundaries and cause a residue problem during the metal etching process. Reducing the time for the high temperature step or lowering the temperature would help minimize this problem. At the same time a cold metal can be redeposited after the high temperature process. Aluminum alloys without silicon content could also be used over a diffusion barrier layer to prevent the silicon precipitates.

Another concern in the multi-step process is achieving repeatable step coverage as well as thin film qualities across a wafer and from one wafer to another. Fig. 5 illustrates the two most important factors, impurity adsorption to the surface of the substrate and the substrate wafer temperature, which influence the reproducibility of the thin film properties produced during the high temperature flow step. Since, as discussed previously, the aluminum flow process relies on the surface diffusion of atoms, the temperature uniformity, the cleanliness of the wafer surface, and impurity levels in a process chamber are key factors determining the repeatability of the process. Localized reactions of the aluminum alloy at the surface, with impurities from either gas phase or dielectric layers, will result in an uneven aluminum flow process on the substrate and the poor reproducibility of process results.

4. Conclusion

Multi-step metallization processes, which comprise at least a cold deposition step and a high temperature annealing or deposition step, have shown promising results for filling the contact/via holes in submicron geometries. Especially, the dep-flow-dep process, which consists of a low temperature deposition in the first module, high temperature flow without deposition in the second module, and finally an additional deposition of the alloy at a low temperature in the third module, showed a good control of the reflectivity and smoothness of the surface as well as the planarization of the deposited alloy in submicron contacts and vias. In addition, the application of this aluminum planarization process to a full CMOS device (Park *et al.* [2]) showed no degradation of electrical properties and enhanced stress and electromigration resistance compared to the conventional one-step aluminum alloy sputter metallization.

The analysis of the mechanisms involved in multi-step process for the contact hole filling concludes that the uniformity of the wafer temperature, the surface cleanliness of the metal film, the impurity levels of a process chamber during the high temperature process are key factors determining the attainment of repeatable process results. Further process optimization and hardware developments for better control of temperature and cleanliness of the wafer surface will surely be a solution for the highly reliable metallization schemes required for lower submicron technology in ULSI.

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