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Effects of Cu Film Texture and Barrier Structure on Cu Grain Growth

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1. Introduction

As a Cu wire width reduces to a deep sub-micron scale in ultra-large scale integrated devices, a large resistance-capacitance delay is one of critical material-related issues. One of the primary factors for the increase in electrical resistivity of the Cu wires is the existence of fine Cu grains. Thus, understanding the mechanism of grain growth in Cu films is essential for reducing the resistivity increase.

In the past decades there have been many investigations on grain growth in Cu thin films [1-3], and both Cu grain growth and Cu texture were reported to be affected by a material type of diffusion barriers: Strong (111)-texture was observed in Cu films deposited on barrier materials such as Ta and Ti, in contrast, some (100)-oriented grains in addition to (111)-oriented grains were observed in those on barrier materials such as W and SiO_2.. The strong (111)-texture suppressed Cu grain growth, and containing the (100)-oriented grains in the (111) grains facilitated Cu grain growth [1-7]. However, comprehensive and quantitative relationship among the Cu grain growth, the Cu texture and the barrier materials is not clear. Thus, in this study, we comprehensively and quantitatively investigated effects of Cu film texture related with barrier materials on Cu grain growth at room temperature (RT).

2. Experimental Procedures

Single-layer barriers of Ta and TaN with 150 nm in thickness and two-layer barriers (Ta/TaN and TaN/Ta with 75 nm in thickness of each layer) were deposited on SiO_2/Si substrates in a radio frequency magnetron sputter system, and followed by about 250 nm- or 10 nm-thick Cu films without breaking the vacuum. Those Cu films were also deposited on barrier-less substrates (SiO_2/Si and ($11\overline{2}$ 0)-oriented sapphire). After the deposition, the samples were kept at RT. The Cu surface was observed by focused ion beam (FIB), atomic force microscope (AFM) and scanning electron microscope (SEM)/energy dispersive X-ray spectroscopy (EDX). The resistivity of the Cu films was measured by van der Pauw method. Texture of the Cu films was investigated by X-ray diffraction (XRD) method: The texture is represented by the area ratio (α) of the $(200)_{Cu}$ peak to the $(222)_{Cu}$ peak. Each peak was fitted by a background and two pseudo-Voigt functions corresponding to $K_{\alpha1}$ and $K_{\alpha2}$ peaks, and the peak area was determined from the area under the fitted curve [8].

3. Results and Discussion

I. Effect of Cu film texture on grain growth (<u>250 nm-thick</u> Cu films)

Figure 1(a) and 1(b) show typical XRD θ-2θ spectra of the $(200)_{Cu}$ and $(222)_{Cu}$ peaks, respectively, for the Cu/SiO_2 sample. Both the $(200)_{Cu}$ and $(222)_{Cu}$ peak areas increased with increasing the keeping time as shown in Fig. 1(c), indicating the Cu grain growth at RT. Similar tendency of keeping-time variation of the peak areas was observed in all the other samples, except for the Cu/Ta sample with the strong (111)-texture. In the sample, the $(222)_{Cu}$ peak area increased with keeping time, whereas no $(200)_{Cu}$ peak was observed even after 150 days or more.

The α values and the resistivity of the Cu films on various barriers are shown in Fig. 2 and 3, respectively, as a function of the keeping time. The α values for the as-deposited Cu samples varied with the barrier materials, indicating the texture of the Cu films were affected by the barrier materials. The α values for the Cu/Ta/TaN, Cu/TaN/Ta and Cu/TaN samples decreased with the keeping time, while those for the Cu/sapphire and Cu/SiO_2 samples increased with the keeping time. The α value change settled down to a specific value after sufficient keeping time, and the specific value for each sample was different. For the Cu/Ta sample, the α value (= 0) did not change at all. Similarly, the resistivity of the as-deposited Cu films varied with the barrier materials, indicating the as-deposited Cu grain size varied with the barrier materials. The resistivity decreased with the keeping time for all the samples, indicating the Cu grain growth at RT. However, the resistivity reduction rates and the minimum values varied with the barrier materials. The minimum resistivity value of about 2 $\mu\Omega$cm was obtained in the Cu/sapphire sample (α~0.9).

Based on these results, quantitative relationship among the resistivity, the α value, and the keeping time was summarized in Fig. 4. The horizontal and vertical axes represent the α value and the resistivity of the Cu films, respectively. The keeping time change is represented by the symbol change as shown in the inset scale. The resistivity of the as-deposited Cu films (around keeping time of 30-50 minutes) generally became large as the α value was larger, indicating the average grain size of as-deposited Cu films became small. On the other hand, the resistivity reduction rate (~grain growth rate) exhibited the maximum value at the specific α value of ~1.0. Similarly, the minimum resistivity value reached in each sample exhibited the lowest value of ~2.0 $\mu\Omega$cm at the specific α value of ~1.0 (Cu/sapphire and Cu/TaN/Ta). Those indicate that Cu grain growth facilitates at the α value of ~1.0. This was confirmed by FIB observation of the samples where grain growth settled down: the average grain size of the samples at RT after 150 days or more was found to be the largest (~500 nm) at the α value of ~1.0 (Fig. 5). This relationship suggests that Cu grain growth rate and the average grain size can be maximized when Cu films consist of a certain amount of (100)-oriented grains in addition to (111)-oriented grains (α = 0.5~1.0), regardless of the as-deposited Cu grain size. Thus, to facilitate Cu grain growth, it is important to control the α value around 1.0 during grain growth at RT.

II. Effect of barriers on Cu film texture (<u>10 nm-thick</u> Cu films)

To clarify how and when the texture of the 250 nm-thick Cu films was determined, texture of the 10 nm-thick Cu films was investigated using the XRD method. The texture was similar to that of the 250 nm-thick Cu films (data not shown). The lateral Cu layer growth was observed in the Cu/Ta and Cu/Ta/TaN samples using AFM and SEM/EDX. While, Cu agglomeration was observed in Cu/SiO_2, Cu/TaN/Ta and Cu/TaN samples, and morphology of Cu islands became coarse as the α value was larger. Typical AFM images of the Cu/Ta and Cu/TaN samples are shown in Fig. 6. Those indicate that the texture of the Cu films was not produced during grain growth, but was made in nucleation. Also, wettability of the Cu films on various barriers plays a key role for determining the texture. The good wettability made a continuous Cu film on the barrier, and internal stress due to difference of thermal expansion coefficient between the Cu films and substrates may lead to formation of strong (111)-texture.

4. Conclusions

The Cu film texture (α values) could be continuously changed by selection of barrier materials. The Cu grain growth rate and the average grain size can be maximized when Cu films consist of a certain amount of (100)-oriented grains in addition to (111)-oriented grains (α = ~1.0), regardless of the as-deposited Cu grain size. The average grain size of the sample (α = ~1.0) was confirmed to be the coarsest. To facilitate Cu grain growth, it is important to control the α value around 1.0 at RT. The texture of the Cu films is concluded to be determined at nucleation, and wettability of the Cu films on various barriers plays a key role for determining the texture.

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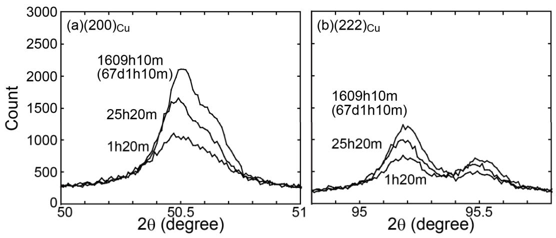

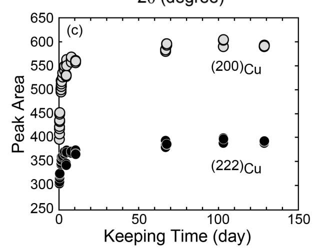

Fig. 1
XRD spectra of (a) $(200)_{Cu}$, (b) $(222)_{Cu}$ peaks for the Cu/SiO_2 sample. (c) Summary of keeping-time variation of the peak areas.

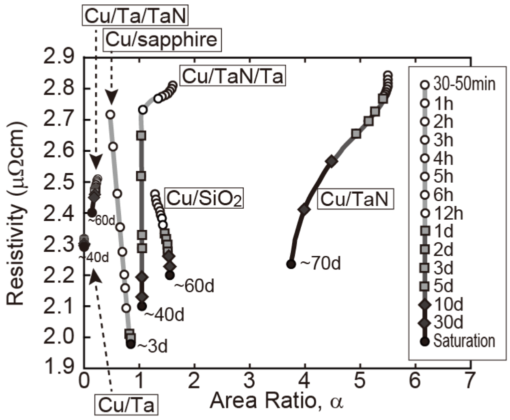

Fig. 4 Relationship among the resistivity, the α value, and the keeping time.

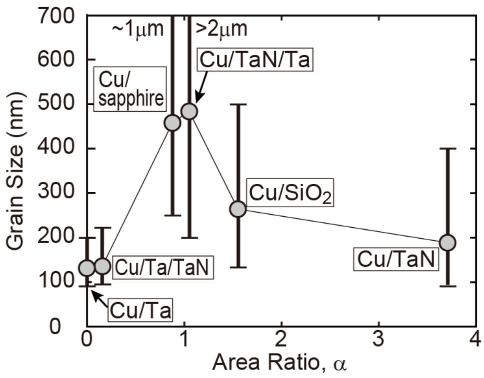

Fig. 5 The average Cu grain size of samples kept at RT after 150 days or more, as a function of the α value.

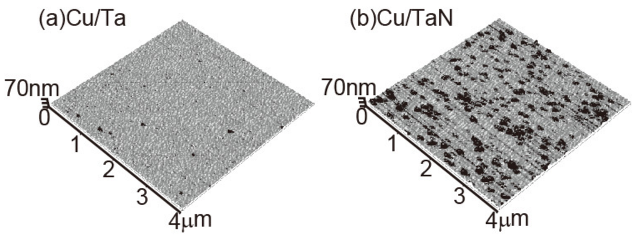

Fig. 6 AFM images of the (a) 10nm-Cu/Ta and (b) 10nm-Cu/TaN samples.

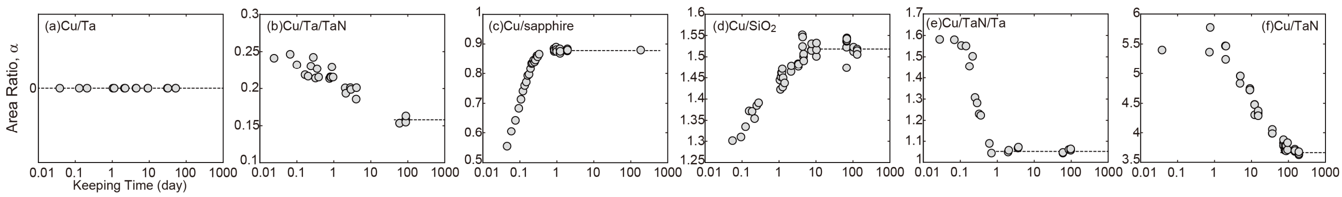

Fig. 2 The α values for (a) Cu/Ta, (b) Cu/Ta/TaN, (c) Cu/sapphire, (d) Cu/SiO_2, (e) Cu/TaN/TaN, (f) Cu/TaN samples as a function of the keeping time.

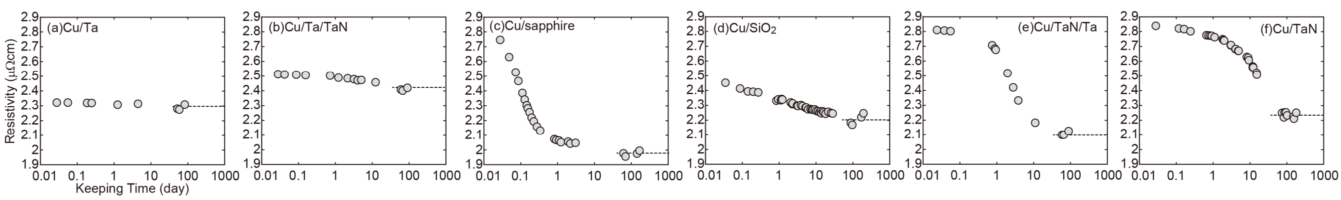

Fig. 3 The resistivity of the Cu films in (a) Cu/Ta, (b) Cu/Ta/TaN, (c) Cu/sapphire, (d) Cu/SiO_2, (e) Cu/TaN/TaN, (f) Cu/TaN samples as a function of the keeping time.