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ABSTRACT

The effects of the Ta underlayer on the adhesion, nucleation, texture, and interdiffusion of overlying Cu films have been investigated using transmission electron microscopy and energy dispersive spectroscopy. Large Cu grains with a strong (111) texture are obtained owing to the heteroepitaxial growth of Cu on a (002) beta-Ta seed layer. Cu reacts readily at 400 °C with Ta to form a thin amorphous interfacial layer that promotes the adhesion of Cu to Ta. The composition of Cu and Ta changes continuously across the amorphous interface. Cu diffuses up to a distance of about 5 nm into Ta, while very little Ta is detected in the Cu layer. Consequently, a thick Ta underlayer is needed to completely suppress Cu diffusion. The extent of the amorphous interface layer remains unchanged even after annealing at 600 °C. A laminate multilayer of alternating thin Ta and Cu layers is intact up to 600 °C, but agglomerates when annealed at 800 °C.

INTRODUCTION

In very large scale integrated (VLSI) devices, the signal delay due to interconnects is no longer negligible compared to intrinsic transistor switching delays[1]. As a result, a more conductive and reliable metallization scheme is urgently needed. Cu metallization is a promising replacement for conventional Al alloys. However, an underlayer will be needed to promote the adhesion of Cu to dielectrics and to prevent the drift of Cu ions through these dielectrics[2]. Some refractory metals and their nitrides including Ta, TaN, TiN, and Ti/TiN have been extensively investigated for this application[3-6]. Among these, Ta was recently reported to seed the growth of (111) Cu[7] which has been shown to provide enhanced electromigration resistance[8] as well as improved adhesion and diffusion barrier property.

In this work, using high resolution and bright field transmission electron microscopy (TEM) as well as X-ray diffraction, the interface between Cu and Ta is analyzed to reveal crystallographic and reaction features at the interface and to evaluate the performance of Ta as an underlayer.

EXPERIMENT

Two types of specimens were fabricated: (1) the Si/SiO$_2$/25-nm Ta/1-μm Cu structure to investigate the interface in question and (2) a 20-ply alternating multilayer of 13-nm Ta and 18-nm Cu on Si/SiO$_2$ to evaluate the thermal stability of the Ta/Cu interface.

The Ta and Cu layers were sputtered *in situ* on thermally grown SiO$_2$ at room temperature. The Cu grain size distribution was determined from plan-view and cross-sectional TEM micrographs in both high resolution and bright field/dark field modes. During TEM sample preparation, the samples were kept below 120 °C to avoid further grain growth since abnormal growth of (002) grains at temperatures as low as 150 °C has been reported[9]. The crystallographic orientations of Cu and Ta at the interface were investigated by electron diffraction. X-ray diffraction was used to

RESULTS AND DISCUSSION

Since the most popular underlayer in semiconductor fabrication is Ti/TiN, the approach of the investigation starts with comparison of Cu films on Ti/TiN and Ta. Fig. 1 shows the bright field images of Cu films deposited on Ti/TiN and Ta. It can be seen at a glance that Cu on the Ta underlayer has larger grains. The Cu film on Ti/TiN has been peeled off at times during the TEM sample preparation. The high resolution electron microscope (HREM) images at the interface between underlayer and Cu shown in Fig. 2 explain clearly the improvement of adhesion with the Ta underlayer. Cu reacts readily with Ta to form an amorphous interface layer with thickness of about 3 nm while TiN/Cu interface has no evidence of interface reaction even after being annealed at 400°C. Since the adhesion of the thin film is determined by the competition between the thermal stress and the physical/chemical bonding, it would be enhanced by the chemical bonding due to the interface reaction such as that between Cu and Ta. The difference in the grain size on the two types of underlayers, however, could not be explained from the HREM micrographs.

The selected area electron diffraction patterns of cross-sectional and plan-view specimens shown in Fig. 3 reveal that Cu on Ta has certain crystallographic orientation relationships not only in-plane, but also in out-of-plane directions. The Cu (111) and Ta (002) planes are aligned parallel to the interface, and both the Cu [2$\bar{2}$0] direction and Ta [330] direction are parallel on those planes. That is $Cu_{(111)[2\bar{2}0]}//Ta_{(002)[330]}$. It is interesting that Cu and Ta have a strong preferred orientation out of plane even though a single Cu grain covers numerous Ta grains. The median
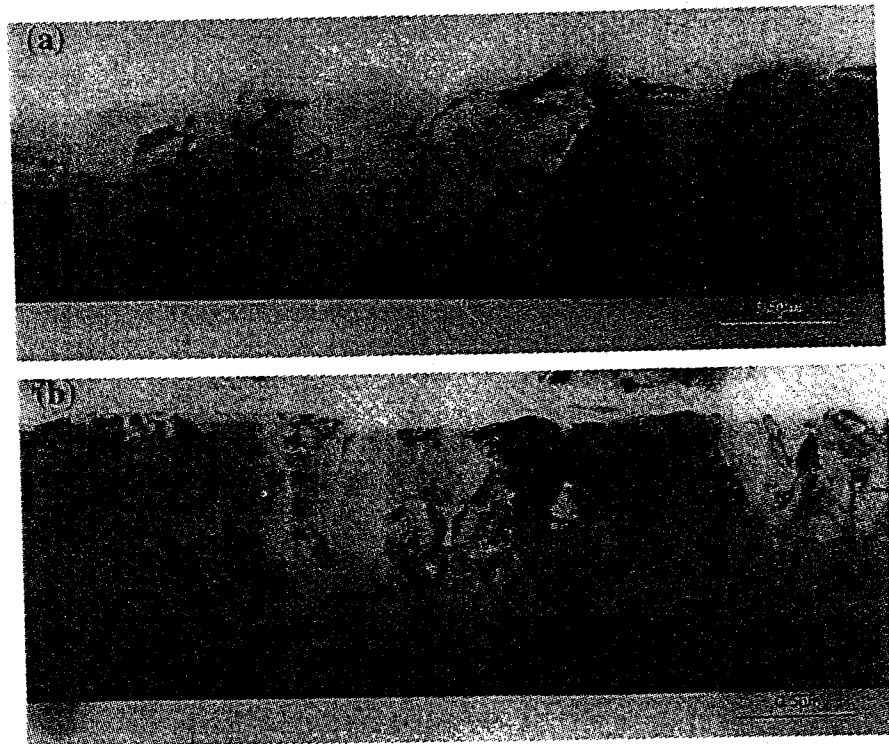

Fig. 1. Bright field TEM images of Cu films grown on (a) tetragonal Ta and (b) Ti/TiN.
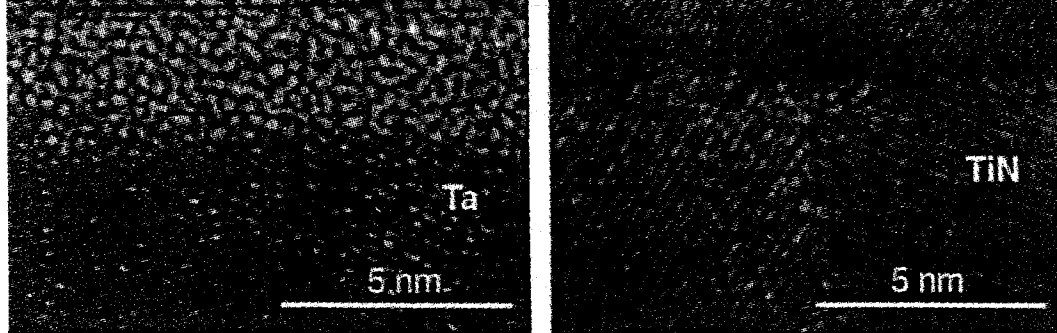
Fig. 2. Cross-sectional high resolution electron microscope images at the interfaces of (a) Ta/Cu and (b) TiN/Cu after anneal at 400 °C.

grain sizes of Ta and Cu are 90 Å and 1600 Å respectively. The large grains of Cu on Ta evidently result from the heteroepitaxial growth of Cu on the Ta underlayer.

An important feature of interface coherency is how the hexagonally symmetric Cu atoms fit onto the tetragonally symmetric Ta atoms. Fig. 4 (a) shows the projection view of atoms in a unit cell of a Ta crystal which has $P4_2/mnm$ symmetry along the c-axis[10,11]. Unexpectedly, the Ta atoms on the (002) plane at elevation of $z/c = 0$ or 0.5 have pseudohexagonal array, and superimpose with eleven of fifteen Cu atoms on its (111) plane as shown in Fig 4 (b). The misfit strain at the interface is 7.6%. The heteroepitaxial growth of Cu also results in a strong texture in Cu which can improve the reliability of Cu interconnects. X-ray diffraction pattern in Fig. 5 verifies the strong (111) texure in Cu Layer.

The formation of the amorphous interface layer observed in Fig. 2 between Cu and Ta is not
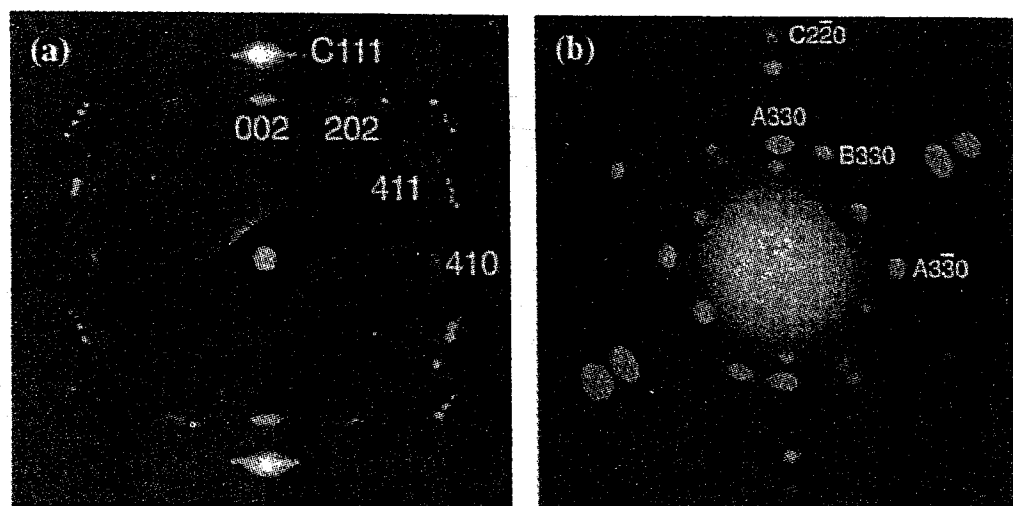

Fig. 3. Selected area electron diffraction patterns of (a) cross-sectional specimen and (b) plan-view sample within a single Cu gran. Prefixes C and 'none' in indices stand for diffraction from Cu and Ta, respectively. A and B in (b) indicate two different sets of diffraction from Ta {330} planes.
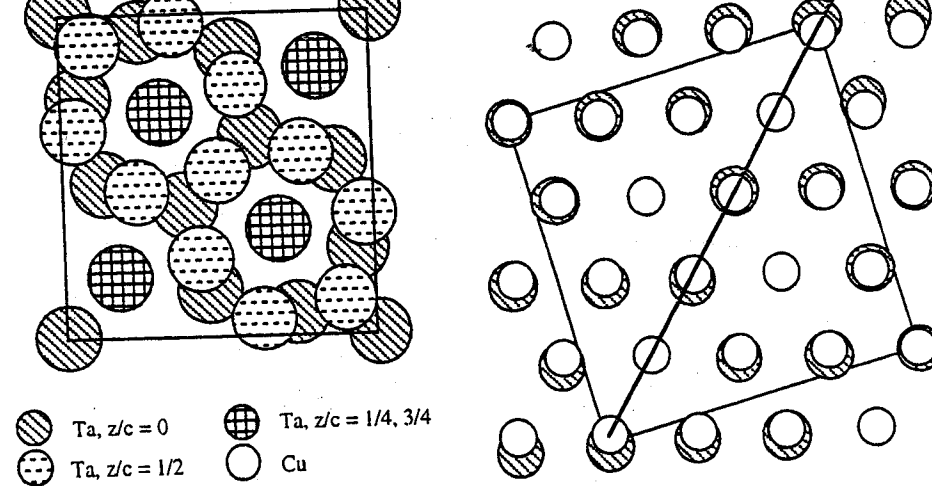
Fig. 4. Schematic projection view of atoms (a) in a unit cell of tetragonal Ta and (b) in mona-
tomic layers of Cu on Ta at the interface. Ta lattice is strained by 7.6% in (b) to illustrate
atomic matching.

clearly understood yet. This is presumably due to a solid state amorphization process which is
common in other metal-metal interfaces such as the Co-Zr system[12]. The composition across
the interface was analyzed before and after annealing at 400 °C by energy dispersive spectroscopy
using an electron probe of 1 nm in diameter. The as-deposited Cu film has a clear interface with Ta
and the composition changes abruptly at the interface as shown in Fig. 6. During the anneal, how-
ever, Cu diffuses at a distance into Ta while little of Ta is detected in the Cu layer. The composi-
tion in the interface layer varies gradually. It is known that the tetragonal Ta has a strong tendency
to align its c-axis normal to the surface[7], and that a channel exists along the c-axis[13] as can be
seen in Fig. 4 (a). Therefore, a relatively thick Ta layer will be needed to block rapid Cu diffusion
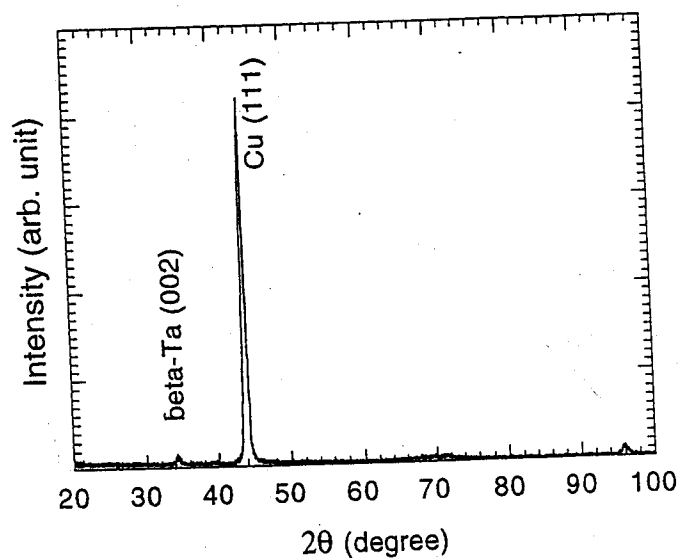

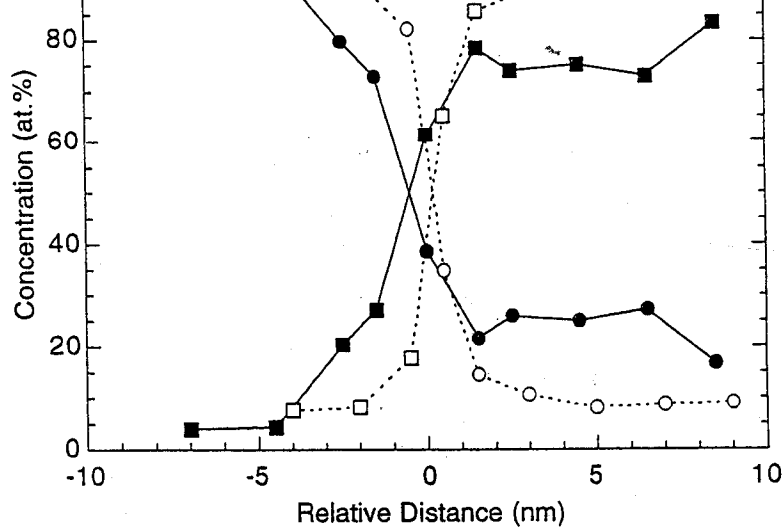Fig. 5. X-ray diffraction pattern of Cu deposited on Ta.

Fig. 6. Composition profiles across the Cu/Ta interface before and after anneal at 400 °C. The electron probe in energy dispersive spectroscopy was 1 nm in diameter.

at elevated temperatures.

According to the thermodynamic study on Cu-bcc Ta system[14], these two metals have little solubility in each other and there is no intermediate phase in between. The formation of an interface amorphous layer and high content of Cu in Ta are probably caused by the fact that Cu is in contact with metastable Ta, not with bcc Ta. A high temperature anneal is essential to examine the stability of the interface between metastable Ta and Cu. A 20-ply alternating multilayer of 13-nm Ta and 18-nm Cu was constructed and subject to heat treatment. Fig. 7 shows a series of bright field TEM images of the composite structure annealed at 600 and 800 °C for 1 hour. The constituent Cu and Ta layers are maintained with clear interfaces at 600 °C. The thickness of the interface layer remains unchanged at 3 nm up to 600 °C. When the multilayer was annealed at 800 °C, two or three Ta layers agglomerate, and the original layered structure is destroyed. This reaction tem-
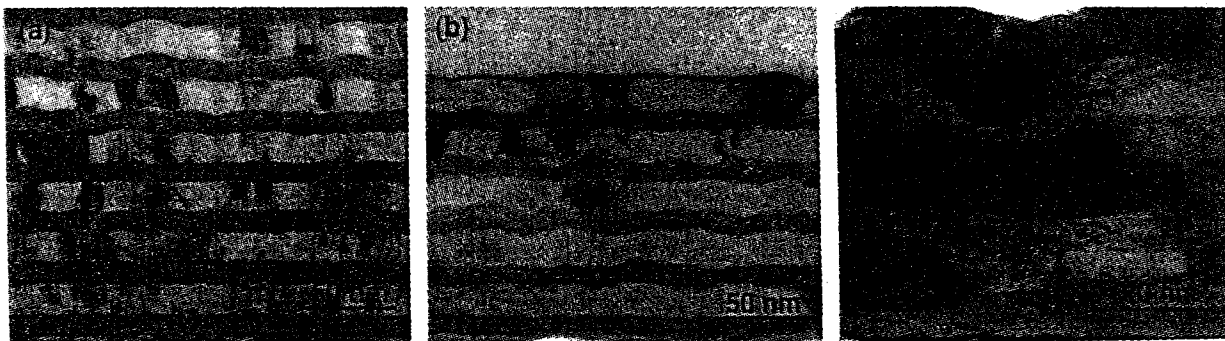

Fig. 7. Bright field TEM micrographs of Cu/Ta multilayers (a) as-deposited, (b) annealed at 600 °C and (c) 800 °C. Dark and bright layers are Ta and Cu layers, respectively.

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