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Low resistivity Ta textured film formed on TaN

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ABSTRACT

Ta films formed on Si(100) and quartz substrates by sputtering technique usually lead to a textured β-Ta with tetragonal crystal lattice. The β-Ta film has a high resistivity. As a comparison, low resistivity α-Ta with cubic crystal lattice can be formed by sputtering on TaN. Crystal study shows that the sputtered TaN film has a preferred (111) growth plane and the α-Ta has a preferred (110) growth plane. Both are textured films. The growth mechanism of the α-Ta on TaN is ascribed to epitaxy.

1. Introduction

In integrated circuits, Tantalum is widely used as metal contact [1]. Ta is also used as diffusion barrier for advanced copper interconnect due to its good adhesion properties between Cu and low-k dielectrics [1,2]. Ta has two stable phases, α-Ta with cubic structure and β-Ta with tetragonal structure. The β-Ta was firstly discovered in sputtered Ta film in 1965 [3]. The β-Ta has a high resistivity of 180 μΩ cm which is much higher than that of α-Ta (24–50 μΩ cm). To reduce the Ta film resistance, several methods have been proposed. Investigation of Ta films grown on Si and sapphire substrates revealed that β-Ta can transform into α-Ta when annealed. But the annealing temperatures needs 300 °C or higher [4,5]. Other methods include α-Ta films grown on Ti [6], on TaN [7], or by N incorporation [8]. However, the fundamental mechanism is not fully clarified.

In this work, X-ray pole figure measurement was conducted on Ta films grown on TaN buffer layer with Si(100) and quartz substrates. Transmission electron microscopy (TEM) was employed to examine the structure details of the Ta/TaN bilayer. The mechanism of α-Ta grown on TaN is ascribed to grain's epitaxial growth.

2. Materials and methods

The substrates were 500-μm-thick n-type Si(100) and 1-mm-thick quartz. All the Si(100) and quartz substrates were firstly cleaned by standard RCA cleaning. The Si(100) received additional dipping in a diluted hydrofluoric acid solution ($HF:H_2O = 1:50$ in vol.) to remove surface oxide. After blown dry by compressed nitrogen gas, all the substrates were sent to vacuum chamber of a TRP-450 sputtering system (S.K.Y. corporation). The base vacuum pressure is 1.0×10^{-4} Pa before each sputtering. The 4-inch sample holder was placed 10 cm away from the Ta target. The Ta target was 99.99% in purity and 60 mm in diameter. Before each deposition, the Ta target was pre-sputtered for 3 min. Ta films were deposited by direct sputtering from the Ta target in pure Ar atmosphere. DC current of 0.30 A and voltage of 310 V were applied to the Ta target during sputtering resulting a Ta deposition rate of 7.3 nm/min. TaN films were deposited from the same Ta target by reactive sputtering in mixed N_2-Ar gas atmosphere. The Ar gas flow and the N_2 gas flow were 3.6 sccm and 3.5 sccm, respectively. Total gas pressure was 0.5 Pa. DC current of 0.30 A and voltage of 435 V were applied to the Ta target during sputtering resulting a TaN deposition rate of 4.8 nm/min. For Ta/TaN bilayer growth, the successive deposition of both layers was simply realized by altering the gas flow rates from $Ar:N_2 = 3.6$ sccm:3.5 sccm to $Ar:N_2 = 7.1$ sccm:0 sccm, with fixed target current of 0.30 A untouched. All the film depositions were conducted at room temperature.

Crystal structure of the films was examined by X-ray diffraction (XRD) and X-ray pole figure measurement with Cu *Kα* radiation in a Panalytical X'Pert PRO diffractometer. The film's cross-section was imaged by TEM. Film resistivity is measured by four point probes according to film thickness data acquired by step profilometer.

3. Results and discussion

Ta film deposited at room temperature usually comprises β-Ta or β-Ta/α-Ta mixture. In our experiment, Ta films were grown on thin and thick TaN buffer layers to show the influence of TaN on Ta growth. Fig. 1 shows the sheet resistance evolution of the samples with various

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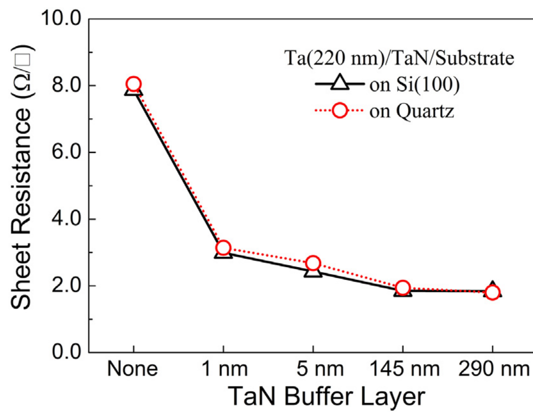

Fig. 1. Sheet resistances of Ta and Ta/TaN bilayers grown on quartz substrate and on Si(100) substrate. The Ta layer is 220 nm in thickness. The thickness of the TaN buffer layer varied from 1 nm to 290 nm.

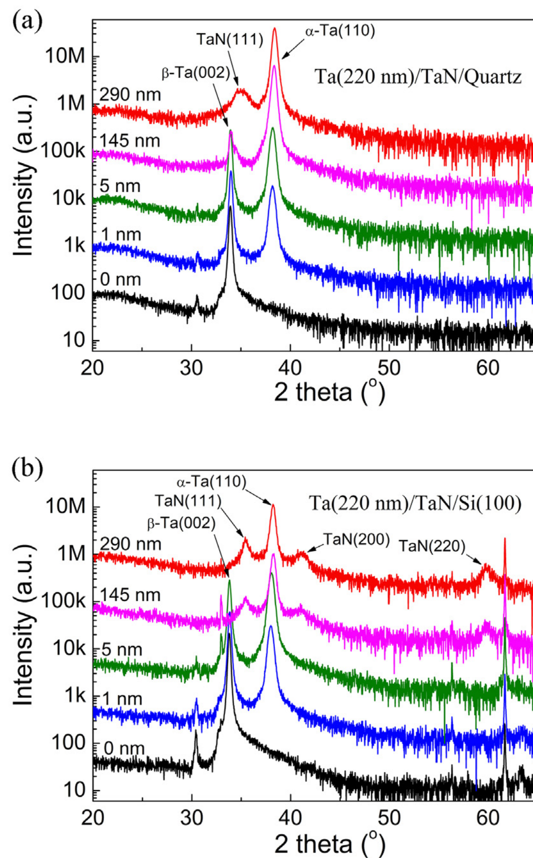

Fig. 2. XRD patterns of Ta film and Ta/TaN stacks grown on quartz substrate (a) and on Si(100) substrate (b). The Ta layer is 220 nm in thickness. The thickness of the TaN buffer layer is varied form 1 nm to 290 nm.

TaN buffer layer thicknesses. The corresponding XRD patterns of the Ta film or Ta/TaN bilayer grown on Si(100) and quartz substrates are shown in Fig. 2.

As calculated from the sheet resistance data in Fig. 1, single layer of 220-nm-thick Ta grown on Si(100) and quartz has a resistivity of 173–177 μΩ cm which is in accordance with the resistivity for β-Ta [3]. No matter the substrate is crystal Si(100) or amorphous quartz, α-Ta phase is undetectable. The very strong β-Ta(002) peak of the Ta film in Fig. 2 indicates a strong textured structure with the (002) plane parallel to the growth surface. The (002) peak is so strong that its corresponding K_β diffraction emerged at $2\theta = 30.6°$. To verify the texture structure,

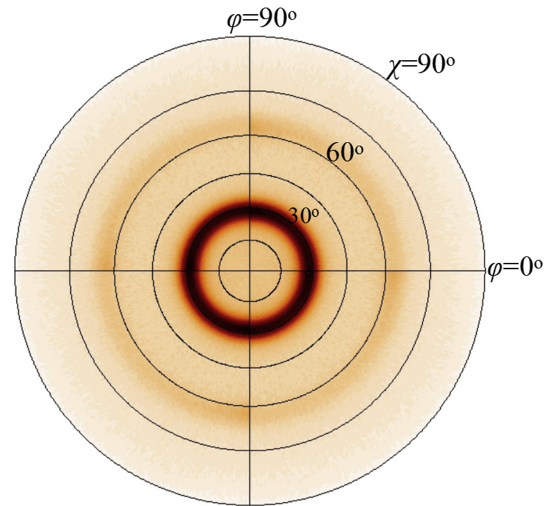

Fig. 3. X-ray pole figure of 220-nm-thick Ta grown on quartz. The 2θ parameter was fixed at 38.62° for β-Ta(202).

the off-axial crystal β-Ta(202) plane was further scanned by pole figure measurement on the (220 nm)Ta/quartz sample. The result is shown in Fig. 3. As known, the tetragonal β-Ta has a lattice constant of a = b = 10.194 Å and c = 5.313 Å [9]. So the ring-shaped (202) feature at around $\chi = 27.5°$ in the pole figure is in agreement with the assumption of the (002) textured β-Ta film. A faint ring-shaped peak around $\chi = 62.5°$ can be recognized and explained by other growth orientations. But the intensity is much lower.

Using TaN as buffer layer resulted in α-Ta growth. As the TaN buffer increased its thickness, the intensity of the β-Ta(002) XRD peak decreased prominently as shown in Fig. 2. At the same time, the α-Ta (110) peak appeared and increased its intensity. For the sample with 290-nm-thick TaN buffer, the peak for β-Ta totally disappeared. Along with change of the Ta metal phase, the film's sheet resistance dropped rapidly from 8.0 Ω/□ to final 1.80 Ω/□. So the resistivity of the 220-nm-thick α-Ta film is calculated to be 39.6 μΩ cm. In the above calculation, we ignore the influence from the underneath TaN because the deposited N-rich TaN has a high film resistivity of 2.66 mΩ cm, which is much larger than that of α-Ta. So the 1.80 Ω/□ sheet resistance is mainly contributed from the Ta layer.

To examine the growth orientation relationship between the successive growth of TaN and α-Ta layers, pole figures of the (220 nm)α-Ta/(290 nm)TaN samples grown on quartz and on Si(100) substrates are scanned in Fig. 4. Both TaN and Ta layers show preferred growth orientations. The preferred grown plane is (111) for TaN and is (110) for α-Ta as judged by the strongest features arising at all centers ($\chi = 0°$, $\varphi = 0°$) of corresponding pole figures. Although the TaN grains may grow with other orientations, as already evidenced by the TaN(200) and TaN(220) XRD peaks shown in Fig. 2(b). But these peaks are weak and sometimes undetectable while the TaN(111) peak is found prominent from sample to sample. For the α-Ta layer, other than the central (110) peak in the pole figures of Fig. 4(b) and (d), a minor ring-shaped feature appearing at $\chi = 60.0°$ can also be identified by diffraction from other {110} planes, including (101), (011), $(10\bar{1})$, and $(01\bar{1})$. Ring shape of the {110} diffraction feature evidenced the fiber texture characteristic of the α-Ta layer.

When TaN is crystallized, its face-centered cubic structure symbolizes the Fm3m lattice in rock salt (NaCl) but with a smaller lattice constant of 4.3399 Å [10]. When viewed along the TaN(111) lattice planes, the Ta atoms or the N atoms are lined up to form periodical hexagonal arrangement as shown in Fig. 5(a). The planar lattice vector of the hexagons is calculated 3.07 Å according to the TaN lattice constant.

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