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SHORT COMMUNICATIONS

Thermal Stability of Thin Amorphous Ta–Si–N Films Used in Au/GaN Metallization

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Abstract—Ta–Si–N Ternary barrier films were obtained by reactive rf magnetron sputtering of a Ta_5Si_3 target in an Ar–N_2 gas discharge. The films were tested as diffusion barriers between Au and GaN layers. The efficiency of these films as diffusion-suppressing barriers is determined by transmission electron microscopy, secondary-ion mass spectroscopy, and X-ray diffraction analysis. It is shown that the diffusion barrier with optimized properties ($Ta_{34}Si_{25}N_{41}$) in an Au/GaN metallization system can be used to advantage at temperatures above 800°C. A correlation between the composition, microstructure, resistivity, thermal stability, and diffusion-suppressing properties of the films is discussed.

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INTRODUCTION

Owing to their unique properties, nitride III–V semiconductors are viewed as a promising material for high-power, high-frequency, and temperature-stable electronic devices [1]. However, a maximal operating temperature (as well as power and frequency) of devices based on III–V nitrides is limited by the lack of stable metallic contacts, rather than by the properties of the semiconductor compounds themselves. Pure metals usually used in Schottky barriers and ohmic contacts react with the semiconductor, causing interdiffusion at the metal–semiconductor interface and, thereby, degradation of the devices operating at high temperatures [2]. Usually, such reactions are prevented by producing a thin diffusion barrier between the metal and semiconductor [3].

The extraordinary combination of the properties of Ta–Si–N films, such as a rather low resistivity, amorphous microstructure (the absence of grain boundaries, which greatly enhance diffusion), chemical inactivity, and thermal stability, makes these materials indispensable for metallization systems in semiconductor devices. In addition, it was demonstrated [4–7] that thin Ta–Si–N films can be used as diffusion barriers in Al and Co metallizations of silicon devices.

Previously [8, 9], we investigated the effect of deposition parameters on the properties and thermal stability of amorphous Ta–Si–N films of different composition, as well as on their performance as diffusion barriers in Ag and Au metallizations of GaAs devices. It was shown that a $Ta_{34}Si_{25}N_{41}$ film 100 nm thick suppresses interdiffusion between Ag or Au and GaAs during annealing at 750 and 800°C, respectively.

In this study, thin $Ta_{34}Si_{25}N_{41}$ films were tested as diffusion barriers between Au and GaN. A relationship between the composition, microstructure, resistivity, thermal stability, and diffusion-suppressing properties of the films is found, and optimal thin-film deposition conditions are determined.

EXPERIMENTAL

Thin Ta–Si–N ternary films were prepared by reactive rf magnetron sputtering of a Ta_5Si_3 target in an Ar–N_2 plasma without intentional cooling or heating of the substrate. The deposition parameters were the following: the gas flow rate ratio during sputtering was N_2/Ar = 10%; the total gas pressure, 0.4 Pa; the power density at the target, 1.7 W/cm^2; and the deposition rate, 38 nm/min. The deposition chamber and process of deposition by reactive sputtering of Ta–Si–N films were described in detail in [8, 9].

The composition of the films (34 at.% Ta, 25 at.% Si, and41 at.% N) was determined by Rutherford backscattering (RBS) of 2-MeV He^+ ions. The thickness of the films measured by a profilometer was about 100 nm. The surface resistance of the 100-nm-thick sputtered $Ta_{34}Si_{25}N_{41}$ films measured by the four-point probe method was approximately 81 Ω/□. X-ray diffraction data indicated that the as-deposited $Ta_{34}Si_{25}N_{41}$ films are amorphous.

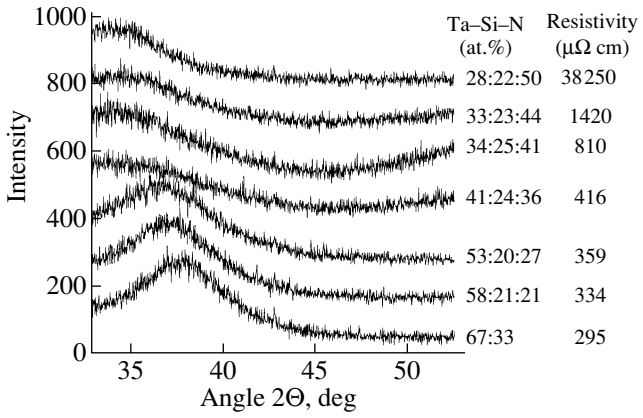

Fig. 1. X-ray diffraction spectra taken of the as-deposited Ta–Si–N films with a different nitrogen concentration. On the right, atomic ratio Ta : Si : N and the resistivity of the films are shown.

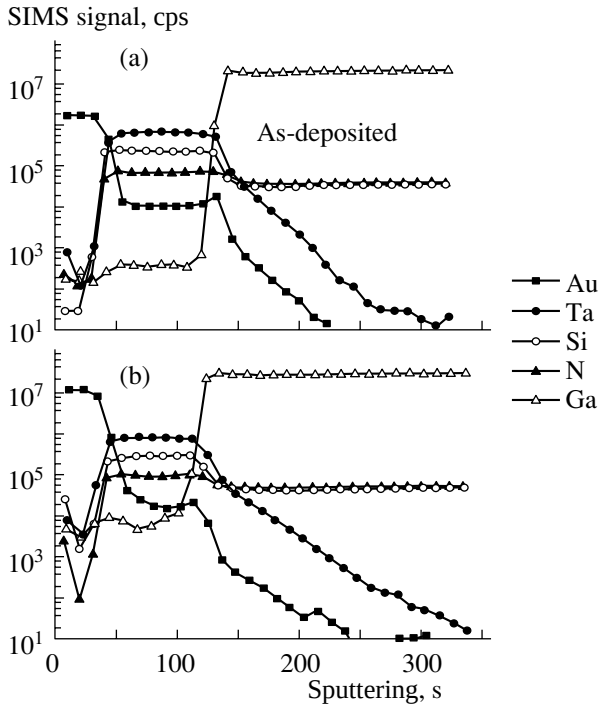

Fig. 2. SIMS element distributions over the depth in the (a) as-deposited $Au/Ta_{34}Si_{25}N_{41}/GaN$ contact structures and (b) the same structures annealed at 800°C for 5 min in the Ar flow.

Magnesium-doped GaN epitaxial layers about 2 μm thick with a carrier density of 1×10^{17} cm^{-3} grown by MOCVD on sapphire were used as substrates for testing the barrier performance of the $Ta_{34}Si_{25}N_{41}$ films included in gold metallization. Before loading to the deposition chamber, the GaN surface was cleaned according to the procedure described in [10]. To characterize the diffusion barrier, $Au/Ta_{34}Si_{25}N_{41}/GaN$ structures were prepared. A 90-nm-thick upper (gold) layer was deposited on a 100-nm-thick $Ta_{34}Si_{25}N_{41}$ film by dc sputtering of a gold target at a power of 70 W in pure argon (0.5 Pa). After annealing for 5 min at 800°C in an argon flow, the samples were investigated by transmission electron microscopy (TEM), secondary ion-mass spectroscopy (SIMS), and X-ray diffraction (XRD) analysis.

RESULTS AND DISCUSSION

Electrophysical Properties of Ta–Si–N Films

In [8, 9], thin Ta–Si–N films with a nitrogen concentration in the range 0–50 at.% were studied. It was shown that, as the nitrogen concentration in the sputtering plasma increases, so do the nitrogen concentration in the films (simultaneously the Ta/Si atomic ratio decreases), (ii) crystallization temperature of the layers, and (iii) resistivity of the films.

According to XRD data, the Ta–Si–N films were amorphous in the as-deposited state: the XRD patterns exhibited a wide diffraction halo typical of the amorphous material (Fig. 1). With an increase in the nitrogen content in the films, the FWHM of the diffraction peak increases and the peak shifts towards lower Bragg angles, indicating a degradation of the short-range order of environmental Ta and Si atoms (the mean atomic spacing increases). The increase in the degree of amorphization correlates with a change in the chemical composition and an increase in the resistivity of the Ta–Si–N films. These findings are corroborated by X-ray photoelectron spectroscopy data obtained in [6, 7], which show that Ta–Si–N films with a high nitrogen concentration feature a combination of Ta–Si, Ta–N, and Si–N bonds. The abrupt increase in the resistivity and the amorphous structure of the high-nitrogen films stem from the fact that the fraction of the poorly conducting amorphous silicon nitride increases, whereas the fraction of well-conducting polycrystalline tantalum nitride decreases with an increase in the nitrogen concentration in the gas phase. These films may be considered as a composite representing a silicon nitride amorphous matrix with tantalum nitride inclusions (see [11, 12]). This model explains why amorphous Ta–Si–N films with a nitrogen content exceeding 40 at.% are thermally stable.

To apply these films as diffusion barriers, the resistivity of the as-deposited films should be less than 1000 μΩ cm [13]. Therefore, the films containing 34 at.% tantalum, 25 at.% silicon, and 41 at.% nitrogen with resistivity of 810 μΩ cm were tested as diffusion barriers.

Barrier Properties of Thin $Ta_{34}Si_{25}N_{41}$ Films

The element depth distribution profiles taken by SIMS from $Au/Ta_{34}Si_{25}N_{41}/GaN$ structures (both as-deposited and subjected to heat treatment at 800°C are shown in Fig. 2. As is seen, any considerable post-

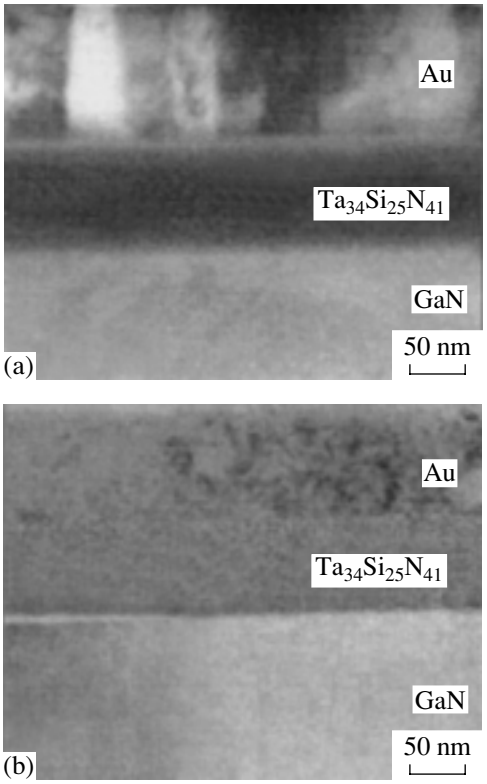

Fig. 3. TEM micrographs taken of the cross section of the Au/$Ta_{34}Si_{25}N_{41}$/GaN samples (a) as-deposited and (b) annealed at 800°C for 5 min in the Ar flow.

anneal redistribution of the elements over the depth is not observed because of the abrupt Au/$Ta_{34}Si_{25}N_{41}$ and $Ta_{34}Si_{25}N_{41}$/GaN interfaces both in the as-deposited and annealed structures. In addition, the shape of the signal from the Au film remains almost unchanged, since Au diffusion into the substrate through the $Ta_{34}Si_{25}N_{41}$ barrier after annealing at 800°C for 5 min is absent. This indicates that the resulting diffusion barrier hinders interdiffusion processes in the Au/$Ta_{34}Si_{25}N_{41}$/GaN contact during thermal annealing.

To gain insight into the thermal stability of the Au/$Ta_{34}Si_{25}N_{41}$ and $Ta_{34}Si_{25}N_{41}$/GaN interfaces, the cross sections of the as-deposited and annealed structures were examined under a transmission electron microscope. Figure 3 shows the micrographs of the cross section of the Au/$Ta_{34}Si_{25}N_{41}$/GaN structure in the as-deposited state and after annealing. The absence of any noticeable changes after annealing at 800°C indicates that the interfaces remain sharp without any evidence of compounding or mixing between the layers. Besides, the Au–barrier and barrier–GaN interfaces, being fairly smooth before annealing, remain such after annealing. Finally, the TEM micrographs suggest that the $Ta_{34}Si_{25}N_{41}$ films are isotropic and amorphous (unlike the Au films, which have a columnar structure) and also that annealing at 800°C does not result in crystallization. This is consistent with the XRD data for the as-deposited and annealed contact structures, which do not show the signs of new phases. Thus, it follows from the SIMS, TEM, and XRD data that thin $Ta_{34}Si_{25}N_{41}$ films sandwiched in between Au and GaN layers subjected to thermal annealing at 800°C may serve as efficient barriers for diffusion.

CONCLUSIONS

Our investigation shows that the structure, composition, resistivity, and barrier properties of Ta–Si–N films are interrelated. Optimal conditions for synthesis of diffusion barriers with a nitrogen content of 41 at.% are found. The microstructure of as-deposited $Ta_{34}Si_{25}N_{41}$ films is amorphous, and the amorphous–crystalline transition occurs at annealing temperatures exceeding 900°C [8]. $Ta_{34}Si_{25}N_{41}$ films of thickness 100 nm and resistivity 810 μΩ cm proved to be excellent diffusion barriers. This is because the amorphous microstructure persists, preventing metallurgical interaction between Au and GaN during annealing for 5 min at 800°C. The aforesaid demonstrates the potential of the films for diffusion barriers in advanced metallizations intended for high-temperature, high-power, and high-frequency electronic devices.

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