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Sputter based Epitaxial Growth and Modeling of Cu/Si Thin Films

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Sputter based Epitaxial Growth and Modeling of Cu/Si Thin Films

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Abstract: Epitaxial copper thin films were deposited by magnetron sputtering. The adatoms during deposition are influenced by deposition parameters which cause variations in thin film properties. XRD and FESEM studies were done to get an insight into the growth mechanisms of the films. 3D island growth attributed to volmer Weber epitaxial growth followed by dewetting due to higher surface energy was observed. A modelling has been done on the epitaxial thin film growth with sputtering process. The parameters during sputtering like, sputtering yield, pressure, temperature, current density, deposition time were related and an attempt has been made to analyse the sputtering process.

Keywords: Epitaxy, thin films, sputtering, modeling.

1 Introduction

The transition metal copper in the form of thin film is applicable not only in electronic industry for interconnects and fabrication of devices but also useful as a bioactive coating required for medical devices as copper is involved in various biological activity like embryonic development, mitochondrial respiration, regulation of hemoglobin etc [1, 2]. Magnetron sputtering is an effective means of depositing nanocomposite as well as epitaxial thin films. The thin film adsorption process during magnetron sputtering is strongly influenced by the deposition parameters. The adatom mechanics can be tuned with the help of deposition parameters changing the thin film properties significantly. Copper thin films have also been deposited by r.f magnetron sputtering on Silicon substrates forming an epitaxy. These epitaxial films are highly favoured as conductor wires because they are free from grain boundary defects. They are also desirable for catalyst layer formation [3]. Deposition conditions like pressure, power, temperature and time have strong influence on the films. By variation of deposition pressure during sputtering, an alteration in the diffusional process occurring on the surface of the Cu thin films have been observed. This transport phenomenon occurring on the surface for copper (Cu) thin films deposited on silicon substrates leads to electro migration which is a major issue in electronic device manufacturing specially interconnects [4].

2 Experimental Details

Copper was deposited on Si (111) and Si (100) substrates by r.f. magnetron sputtering. The r.f. power was kept constant at 250 W with reflected power around 20 W at room temperature. The chamber pressure and deposition time were varied. The collisions taking place between the sputtered adatoms and the gas molecules in the chamber will depend upon the gas flow inside the chamber. The adatoms on reaching the substrate surface undergo diffusion to become thermodynamically and energetically stable. They also gain kinetic energy from the substrate temperature. XRD and SEM studies were done to throw some light on their growth mechanisms affecting their properties.

3 Results

3.1 XRD Studies

XRD studies were performed on the thin films as well of the Si (100) substrate [Fig 1]. The base Si (100) showed a characteristic peak at 68°. No major change was observed in the diffraction plot of Cu/Si (100) films which were deposited at 5 Pa pressure for 60s. The intensity of the peak coming from the base silicon was however much lower for films deposited for 300 s. An explanation for the lowering of the intensity could be the vibrations of the surface atoms about their equilibrium position and as a result the exact Bragg condition was not met. Another explanation could be the higher copper deposition reducing the substrate effect. The peaks due to copper were however visible only for films deposited at 5Pa pressure for 2 hrs. Changing the pressure to 1Pa while keeping the time of deposition again

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to 2hr interestingly showed absence of any major peak either from Cu or Si showing chamber pressure playing a significant part in the surface properties of the film which was clear on performing the microscopic studies.

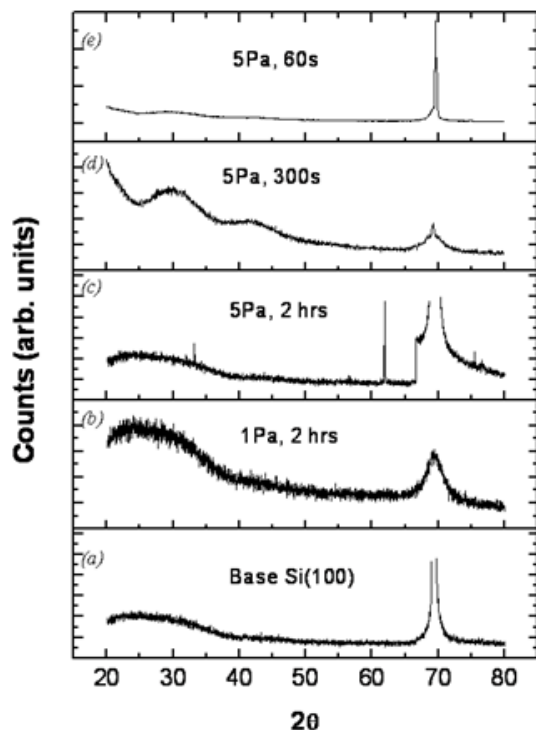


Figure 1. XRD of Cu/Si at different deposition conditions

3.2 FESEM studies

The FESEM studies for Cu/Si (100) are shown in Fig 3. The micrograph of the base silicon (100) surface is shown in Fig 2a. The deposition pressure and time are given on each micrograph. Fig 2c on the other hand shows the surface of Cu deposited on Si (100) for 1 hr at 1 Pa pressure at room temperature. The Cu nuclei primarily grew on silicon by the Volmer-Weber mode which was evident from the 3D spherical island growth for the films deposited for 60 s and 300s at 5 Pa pressure. This type of growth arises when the film atoms are more strongly bound to each other than to the substrate [5].

During deposition, the degree of crystallinity increased with deposition time and agglomeration and coalescence of grains took place. The irregular grain shape and orientation is attributed to the inhomogenous nature of sputtering process leading to larger size of the sputtered particles as well as the use of polycrystalline target which has an inhomogeneous microstructure. Single crystal targets however give homogenous films as the sputtered species have more uniform size and energy [3]. The substrate temperature in this case is also significant as the adatoms coming to the surface of the substrate acquire kinetic energy from the substrate temperature and may result in polycrystalline film. A higher substrate

temperature may however lead to accelerated film oxidation [3]. Studies on the effect of Ar pressure on the microstructure and also on the formation of nanotwinned Cu films can be found in the literature [6, 7]. An abstract of the above discussion has been published [8].

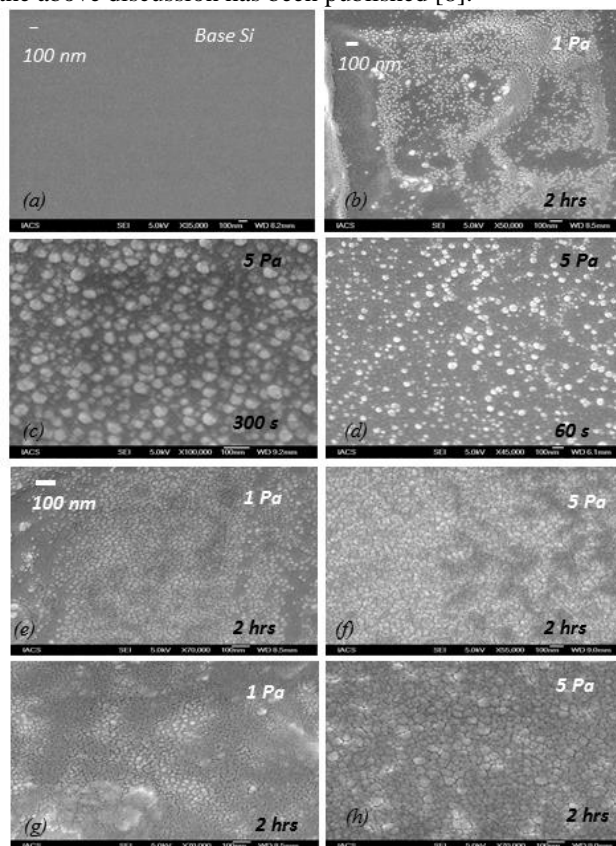


Figure 2. FESEM studies of base Si (100) and Cu/Si (100) deposited at different conditions

The islands formed as observed in the SEM image may also be attributed to the phenomenon of dewetting and occurred due to larger surface energy of Cu compared to the substrate. Similar phenomena have been reported previously but with ion beams [9, 10]. This phenomenon of dewetting in metallic liquid thin films has been reported to be due to nucleation and growth of holes or instability against thermally activated surface waves [11].

3.3 Computational Studies

Sputtering is an effective means of depositing thin films. It based upon hitting a target (cathode) with energized ions to eject out adatoms from it. These adatoms get deposited on the substrate and form the film. The number of adatoms coming out per incident ion is called the sputtering yield. An inert gas usually argon is introduced in an evacuated chamber and ionized. A plasma is formed in the process of ionization. The atomic density in plasma is usually of the order of 10^{-18} per m^3 . The sputtering rate i.e the amount of target materials sputtered per unit time is given by $zt = M/(rNAe) S j p$. where M is molar weight of the target

[kg/mol]; r is the density of the material [kg/m³]; NA is the 6.02×10^{26} 1/kmol; (Avogadro number); e is the 1.6×10^{-19} As (electron charge); S is the sputtering yield (atom/ion) and j_p : primary ion current density [A/m²]. This rate divided by atomic diameter gives us the rate of sputtering in terms of atomic layers (AL) per second [12]. The adatoms sputtered from the target undergoes collision with the gas molecules was then multiplied with $\exp(-x/L)$ to get rough estimate of the deposited atomic layers per second. L (cm) is the mean free path of the sputtered atom which is related to the sputtering pressure P (Torr) and the molecular diameter D_a of the sputtering gas (372 pm for Ar) $L = 2.303 \times 10^{-20} T / (P D_a r^2)$ where T is the deposition temperature and x (cm) is the distance traversed by the adatom for deposition which was taken as 30 cm considering the target the substrate distance[13].

For copper (Cu) which has molar weight of 63.5 g/mol, density of 8.96 g/cm³, sputtering yield of 1 for 1keV Ar ion. The radius of tungsten atom is 0.128 nm. A program was written and the parameters which were varied to get a variation in the deposited ALs are given in Table 1

Table 1: The parameters with their ranges which can be varied during the sputtering

S.No	Parameter	Symbol	Range
1.	Sputtering Yield	S	0.5- 2.5
2.	Current density	J_p	1-25 (mA)
3.	Target to substrate distance	x	30 – 100 (cm)
4.	Sputtering time	t	1.0 -10.0 (s)
5.	Sputtering Pressure	P	$10^{-2} - 10^{-6}$ Torr
6.	Sputtering Temperature	T	300 – 700 K

Each parameter was varied independently keeping the other parameters with a constant to see the effect on the deposition. The deposition pressure P was kept at 10^{-2} Torr, deposition temperature at 300K (RT) and deposition time t was for 30s. The variation of Atomic Layer depositions with sputtering yield at different deposition time is shown in Fig 3. The plasma current density in this case was kept fixed at 1 mA/cm². It can be observed that the rate of sputtering increases with increase in deposition time

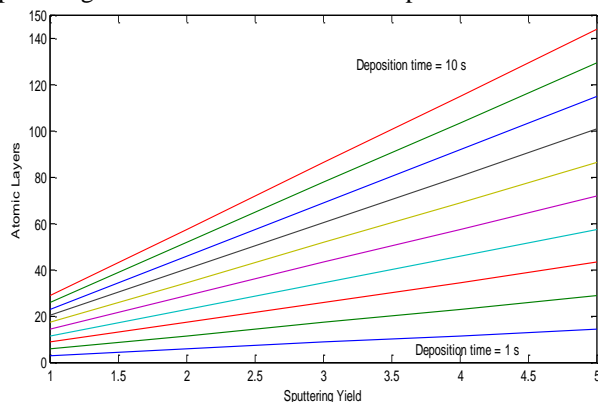


Figure 3: Atomic layers deposited with sputtering yield at different deposition times.

The variation of Atomic layers deposited with source to substrate distance is shown in fig 4(a). The plot attains saturation after an initial increase. The rate of deposition depends on the ratio of mean free path of the adatoms and the source to target distance or working distance (WD). The ratio is also known as Knudsen number (Kn) in some instances. Kn should have a value > 1 for effective deposition to avoid adatom collisions and as a result loss of energy.

However there seems to be also a lower limit to the WD mainly due to the fact that the secondary electrons created during sputtering which are accelerated back across cathode dark space into a negative glow region where additional gas ions are created and the plasma is sustained. The substrate therefore should be kept after the negative glow region or in the anode dark space. Also in terms of angle of deposition it is reported that the sputtering is usually at its peak at an angle of 60°. The change of WD by changing the substrate position may affect the angle. A decrease in deposition rate with increasing WD as well as variation with angle of contacts is reported [14-16].

We have used a pressure of $1e-3$ Torr. For different pressures however different plots are obtained as shown in fig 4(b). It shows that for lower and higher pressure the atomic layer deposition attains a constant value and is partially independent of the source to substrate distance. For pressures in the range of $1e-3$ and $1e-4$, the variation is more pronounced. The explanation behind this result is the collisions the adatoms encountered during deposition. At low pressure or high vacuum, the mean free path of the adatoms is very large and thus the adatoms undergo very less collisions and so variation of target to substrate distance is insignificant. At higher pressure and lower vacuum conditions the mean free path being small, the adatoms undergo severe collisions which also makes the source to substrate distance insignificant. A decrease in deposition rate with increase in gas pressure being more pronounced at lower working (target to substrate) distance has been reported by reported earlier [17].

The Atomic layers decreased steadily with increase in temperature which can be attributed to the stress arising in the films due to increase in temperature causing lower adhesion with the substrate. In practical situation the variation is not so meticulous as lot of other factor like diffusion, coalescence of adatoms, thickness of films comes into the picture which requires further computation modeling. The increase in atomic layers deposited with current density is obvious from the fact that an increase current density usually leads to higher sputter rates.

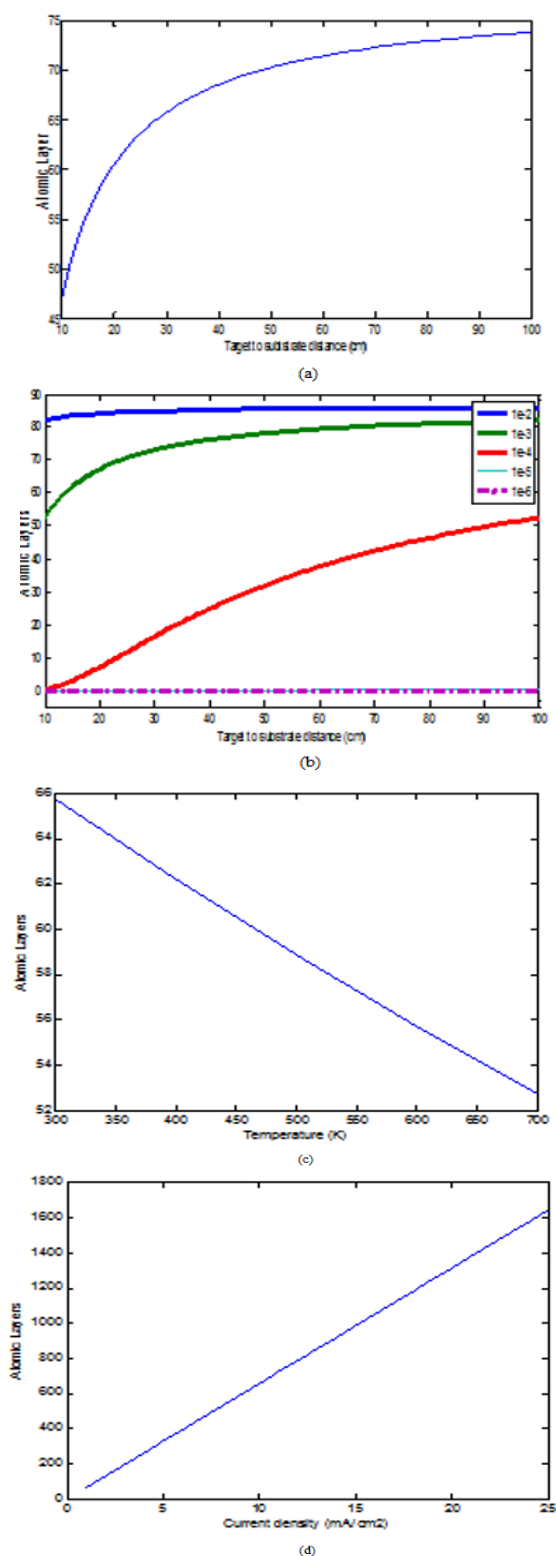


Figure 4: Atomic Layers deposited vs. (a) target to substrate distance (b) vs. target to substrate distance at different pressures Atomic Layers deposited vs. (c) temperature and (d) current density

4 Conclusions

XRD and SEM studies provided an understanding of the growth mechanisms of the films. The Cu nuclei growth primarily took place on silicon by the Volmer-Weber mode which was evident from the 3D spherical island growth for the films. XRD studies showed an optimized pressure of 5 Pa and deposition time of 2 hrs giving a high intensity of diffraction peak corresponding to Cu. Computational studies provided a model for the atomic layer variation with sputtering yield, working distance, pressure, temperature and current density which tallied with experimental results.

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