Thin Solid Films 587 (2015) 3–7

Contents lists available at ScienceDirect

Thin Solid Films

journal homepage: www.elsevier.com/locate/tsf

The effect of negative ions from the target on thin film deposition in a direct current magnetron sputtering system

Min Young Hur, Jin Seok Kim, Hae June Lee *

Department of Electrical Engineering, Pusan National University, Busan 609-735, South Korea

ARTICLE INFO

Available online 13 March 2015

Keywords:
Magnetron sputtering
Negative oxygen ions
Particle-in-cell simulation

ABSTRACT

The effect of the negative oxygen ions in direct current magnetron sputtering on the thin film deposition is investigated with a two-dimensional particle-in-cell simulation with the variation of argon gas pressure ranging from 1.33 to 6.67 Pa (10 to 50 mTorr). While the plasma density increases with the increase of gas pressure, the total amount of the negative oxygen ions emitted from the target surface does not change significantly with respect to the gas pressure. The amount of high energy O^- ions having small incident angles on the substrate decreases with increasing gas pressure especially at the target erosion region. On the contrary, the amount of low energy O^- ions having large incident angles on the substrate increases with increasing gas pressure especially at the center region. The tendency for the change of spatial resistivity of ZnO thin films with respect to gas pressure can be explained with the simulation results.

1. Introduction

There are many methods for the deposition of transparent conducting oxide (TCO) which is popularly used in display and solar cell devices. The main goal of searching high quality TCO films is to achieve a lower resistivity and a higher transmittance in the visible range. Both direct current (DC) and radio frequency (RF) magnetron sputtering systems are widely used for TCO deposition because it is possible to get high homogeneity and good film quality even at low deposition temperature [1–7]. The electrical resistivity (or electrical conductivity) is an important check-up parameter to make a high quality TCO. However, in the thin films deposited by using magnetron sputtering, high electrical resistivity is measured sometimes [4–7], which is estimated being caused by negative ions such as O^-. They are sputtered from the target and accelerated by the electric field and go to the substrate with energy as high as the voltage drop between the substrate and the target. Near the target, plasma sheath potential gives high energy to negative ions which are delivered to the crystalline TCOs. Therefore, it is important to investigate the flux, energy, and angle distributions of the negative ions on the substrate.

In this paper, spatial distribution and energy and angle profiles of negative oxygen ions on the substrate are investigated for DC magnetron sputters using a two-dimensional particle-in-cell (PIC) simulation [8] for the variation of argon gas pressure. The simulation methods are described in Section 2 followed by results and discussions in Section 3. Finally, conclusions are summarized in Section 4.

2. Simulation methods

Fig. 1(a) shows the structure of a DC magnetron sputtering system simulated in this study. There are a target on a permanent magnet and a substrate in the opposite side. The rectangular region drawn with the dashed line is the simulation domain in two-dimensional Cartesian geometry. Only the static magnetic fields are considered because the induced magnetic field by plasma motion is negligible. An open source software, Finite Element Method Magnetics (FEMM), was used to calculate the magnetic flux density by the permanent magnet. The magnetic field profile calculated by FEMM is used as input data to calculate the particle motion in the PIC simulation. Fig. 1(b) shows the distribution of the magnetic flux density. Color contour means its magnitude and the direction is represented by arrows. The average value on the target surface is about 0.025 T.

Three steps are processed in the simulation: (1) a PIC simulation of plasma dynamics, (2) calculation of sputtering yields from the ion bombardment on the target, and (3) the trace of negative oxygen ions from the target to the substrate using a PIC simulation. To calculate the electric field, the finite difference method is used and the periodic boundary condition is applied at the left and the right side boundaries. The electrostatic potential is set to zero on the substrate and the target is connected to a DC current source [9].

Sputtering yield mainly depends on the energy and the angle of the incident ions bombarding on the target. In general, sputtering yield increases with the increasing ion energy and the incident angle. In this paper, ZnO target is considered, in which the compound material is difficult to measure the sputtering yields. From the Sigmund theory [10], sputtering yield is calculated through the mass and atomic number of target atom and bombardment ion species. Sputtering yield of compound

* Corresponding author.
E-mail address: haejune@pusan.ac.kr (H.J. Lee).

http://dx.doi.org/10.1016/j.tsf.2015.03.019

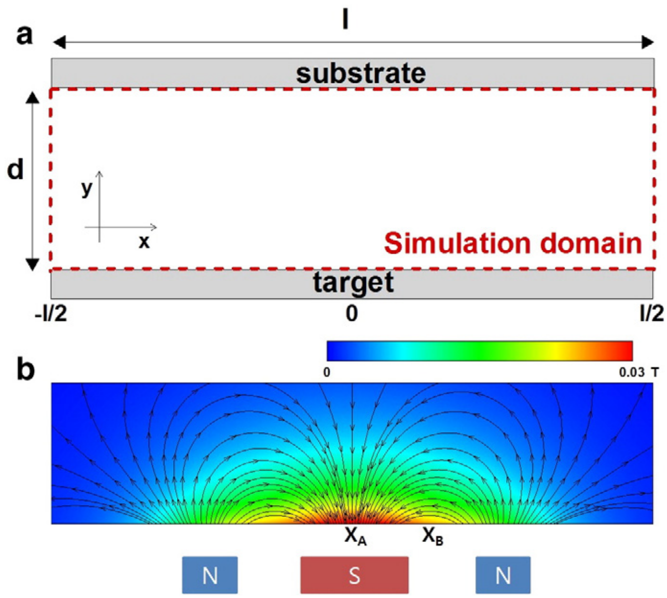

Fig. 1. Shown are (a) the simulation domain of a magnetron sputter and (b) the calculated magnetic flux density in it. The contour plot shows the magnitude of the magnetic flux density, and the arrow shows the direction of the vector field.

material target is calculated by the combination of the mass and the atomic number of compound material [11]. However, Sigmund's theory is applicable only for the ion bombardment energy higher than 250 eV [12]. A modified formula for low ion bombardment energy was calculated from fitting parameter for different target atoms by ion bombardment experiment [12,13]. No data has been reported about ZnO target because it is difficult to measure the sputtering yield on compound material target, nor the Sigmund theory is applicable to the compound. Therefore, we assumed that the sputtering yield of ZnO is similar to that of copper because many elemental solid matters have similar tendency. Cu (29) has similar atomic number to Zn (30). The Yamamura formula [12,13] was used in order to calculate the sputtering yield.

Two assumptions are used to simulate the sputtered particles from the target to the substrate. Firstly, only oxygen atoms which become negative ions are considered. They are negatively charged by electron attachment as soon as they are sputtered. Secondly, sputtered negative oxygen ions collide only with argon atoms rather than Zn, O, O_2 and other impurities because Ar is the dominant gas species in the model. The collision cross section of O^- ions with Ar was estimated from the previous report on cross sections and transport properties of negative ions in rare gases [14].

As shown in Fig. 1(a), d is the gap distance between the substrate and the target, and l is the length of the target. In this paper, d and l are fixed to 6 cm and 25.6 cm, respectively. The width of the magnet is 1.5 cm for the N pole, and 3 cm for the S pole. The distance from the center of the N pole to the center of S pole is 5.65 cm. The applied DC current is fixed to be 0.5 A. Uniform argon background gas is used with a gas temperature of 300 K. The gas pressure ranges from 1.33 to 6.67 Pa (10 to 50 mTorr).

3. Results and discussions

The plasma density in the magnetron sputter is maximized where the magnetic flux lines are parallel to the target surface by the magnetic mirror effect. Because the ionization occurs at the region of high electron density, argon ions have the same density distribution as the electrons although argon ions are not magnetized with 0.025 T. Fig. 2 shows the change of argon ion density with the variation of gas pressure at $x = 3.35$ cm where the highest plasma density is observed. The ion density increases with increasing gas pressure because of increasing ionization. The density is high near the target surface where electrons are effectively confined by the magnetic field, and it decreases with increasing distance toward the substrate.

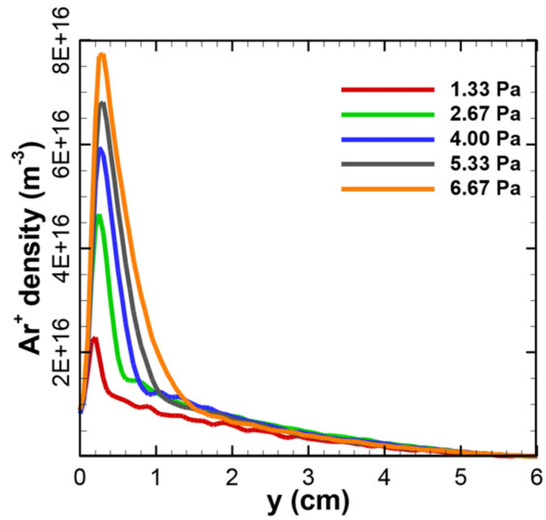

Fig. 2. Argon ion density profiles at the peak density position ($x = 3.35$ cm) for each pressure.

Fig. 3(a) shows the relative potential difference with respect to the target potential with the variation of gas pressure at $x = 3.35$ cm. The target is negatively biased and the substrate is grounded. The potential difference between the target and the substrate is almost the same as

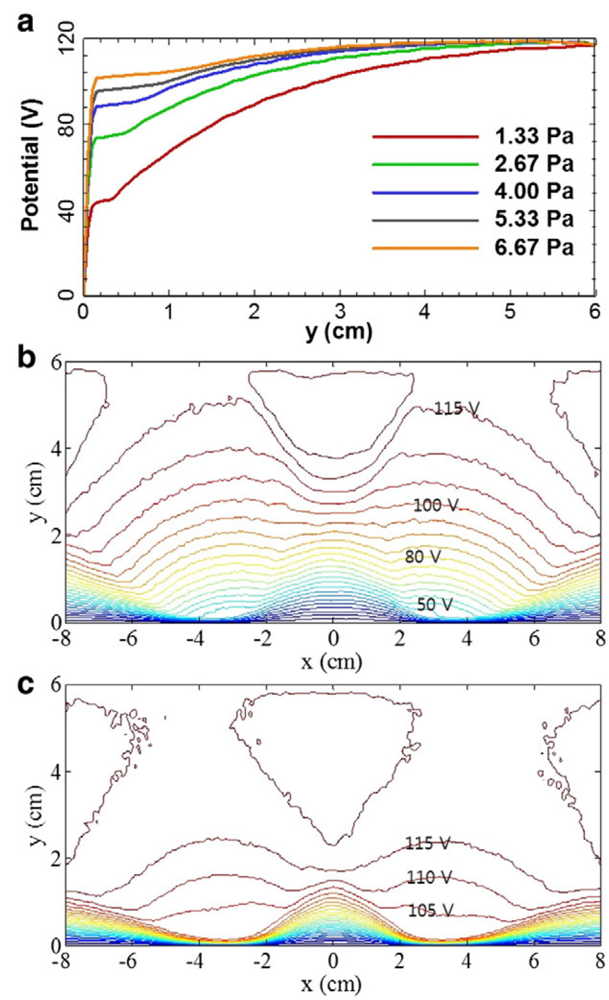

Fig. 3. Shown are (a) potential differences from the target surface at the peak density position ($x = 3.35$ cm) for each pressure, (b) two-dimensional contour plots of the electrostatic potential for 1.33 Pa, and (c) for 6.67 Pa.