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Composite Targets and compositional inhomogeneities in sputter deposited thin films

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Abstract

A numerical study of the compositional distribution of thin films from two components targets has been carried out. The study, based on the string model, considered both the composite nature of the targets and the deviation of the angular distribution of some sputtered atoms from the normal co-sinusoidal distribution function. Large improvements on the compositional homogeneity of the films could be obtained by carefully selecting the number, area and placement of the chips (segregates) on the host target surface.

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1.0 Introduction

The stoichiometry of films deposited from multicomponent targets has been addressed by a number of works [1] – [3]. This is perhaps to the degree of significance the stoichiometry has on the application the films are studied or fabricated for. To control film stoichiometry, many parameters need be carefully considered. One of the most significant is perhaps the uniformity or homogeneity of the target. This is especially difficult with some alloys and mixtures in which constituents segregate out in patches.

Another problem with film compositional homogeneity – that is not limited to composite targets but to almost all multi-component targets is the difference between the angular distribution of the atoms eject from the target [4]. This paper attempts to numerically determine the degree of compositional in-homogeneity of films deposited from a two component campsite targets. The compositions expected of the films are mapped out as functions of the substrate coordinates.

2.0 Calculation

The profiles were calculated on the basis of the string model [5]. In the model, the growing film surface is considered to be given as a string connecting many points as illustrated in Figure 1. The model assumes that the mean free path of the sputtered atoms is far longer than the target to substrate separation and that the sticking coefficient of sputtered atoms is one. The films grow towards the atom flux and increase in thickness at a rate proportional to $\cos\psi$, where ψ is the angle of incidence (between the atom flux and the substrate normal.) It is further assume that the thickness of the growing film at any point P on the substrate comes from the contributions of all components of the target at their relative proportions

In the initial sections of this paper, it is further assumed that atoms are sputtered isotropically (following a co-sinusoidal distribution.) The effects of anisotropy in the angular distribution of sputtered atoms are considered later in two known distribution functions were incorporated.

Based on this model, the film growth at point P on the substrate due to contribution from atom specie A of the target is

$$\vec{r}_A = \int \frac{A_A(\psi) N_A E}{L^2} V_A dS\hat{e} \qquad (2.1)$$

where $\hat{e}$ is a unit vector directed from the areal element dS of the target to P and $D_A(\psi)$ is the angular distribution function of component A. Depending on the geometry and configuration of the sputtering equipment, targets are not normally sputtered at the same rte across their surfaces. The symbol E standing for the erosion rate of the target, is a function that gives the relative depth distribution of the target. As ours is a pure numerical study (not specific to any particular target) it is used here to specify the compositional in-homogeneity of the target. dS is an areal element of the target surface while V_A, is the volume of the atom of element *A* of the target. The parameters *L* and *N* give the target dimension and composition respectively. *L* is the distance between the substrate position P and the target position from where the atom is sputtered. The parameter *N* specify the target composition. It gives, say the ratio between the components of the target. For example, 0.04 for Cr in A_80B_20 target. With the film growth given by the above equation, the film composition at point P is determined for a two component target by the ratio

$$\left(\frac{\frac{t_A}{V_A}}{\frac{t_B}{V_B}}\right) \tag{2.2}$$

where t_A and t_B of the material A and B deposited at P respectively. These are given as the normal component of the film growth

$$t_A = \bar{T}_A \cdot \hat{n} \tag{2.3}$$

Geometry

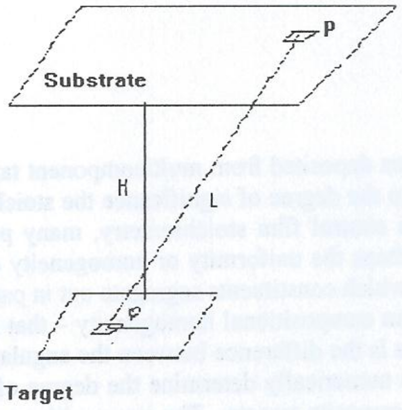

Figure 1: Geometry of the sputtering problem. The film thickness at P is calculated as coming from contributions of the multi-components of the targets sputtered from the entire target surface.

The calculations for the film growth descried are carried out repeatedly for small areal elements *dS* of the target and layer-by-layer deposition is carried out until the final film thickness reaches a desired value.

3. Results and Discussion

The calculations described above shows that the total film thickness is stopped at 100 mm. The results for three chip setting are illustrated in Figures 2 – 4. When three chips of the material making the second component B of the two component $A_{80}B_{20}$ were considered to be placed on the host target, that is material A, the composition profile is as shown in Figure 2. In both Figures (a) and (b) the composition of the B component could seem to concentrate around the centre. When a smaller substrate is used the composition of the film collected by it could vary greatly depending on where in the flux of the atoms it is. The composition when the chips were arranged along a surface diagonal of the target (b) is relatively more uniform than when they were placed along the long (horizontal) axis of he target surface (b). The peak composition of both (a) and (b) are 1.53 atomic percent and 1.48 at.% respectively. That is a substrate collecting atoms from the flux that is towards the centre will have composition of A material less than expected by some 1.53 at.% and that of component B higher by about the same percentage.

When five chips were considered placed on the target surface, the compositional profile is modelled in Figure 3. Figure 3(a) shows the profile when the chips are arranged one of the diagonals of the target surface. Both arrangements could not be seen to very much improve the compositional homogeneity of the films.

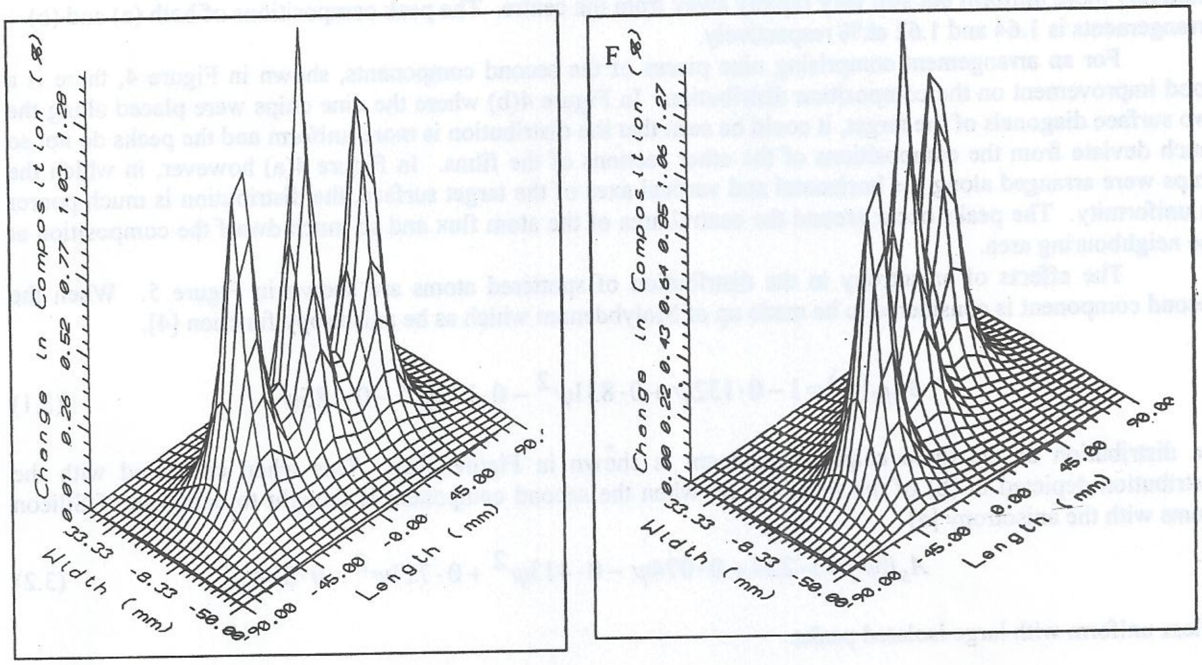

Figure 2(a) Figure 2(b)

Figure 2: Model profile of a film deposited from a two component composite target in which three pieces of one component are placed (a) along the long axis of the target surface and (b) along one of the surface diagonals.

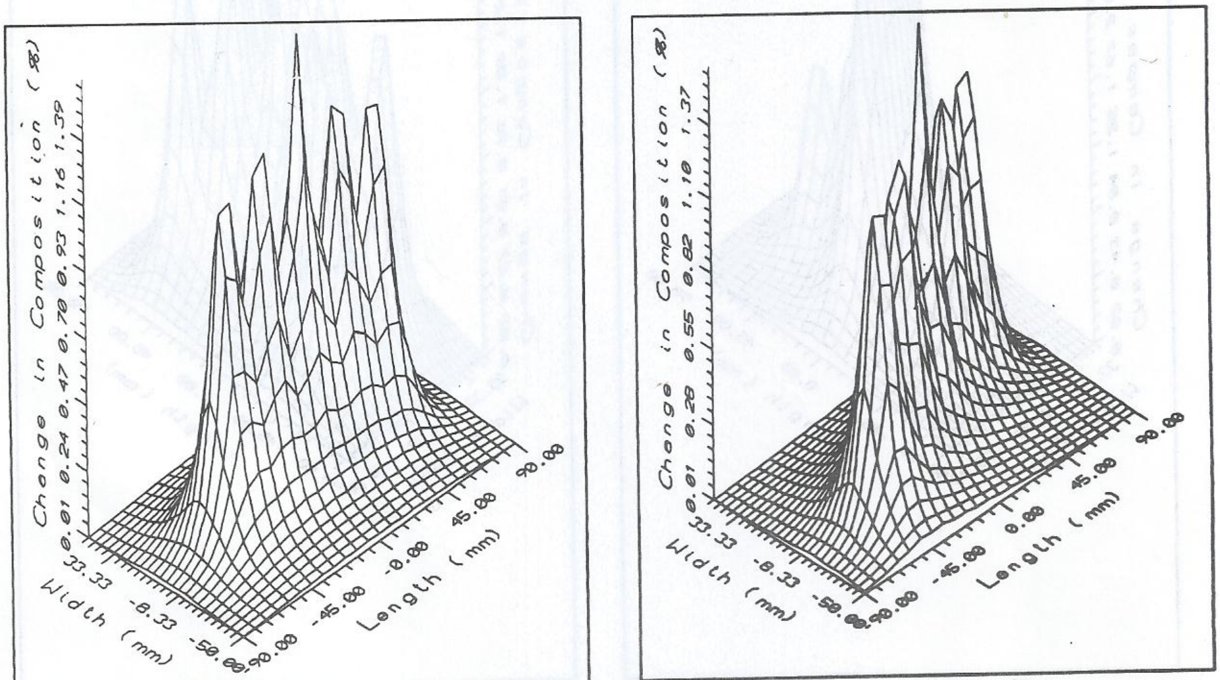

Figure 3(a) Figure 3(b)

Figure 3: Model profile of a film deposited from a two component composite target in which five pieces of one component are placed (a) along the horizontal and the vertical axis of the target surface and (b) along the two surface diagonals.

Along the central area of the flux the composition (although higher for the second component) is relatively more uniform but still vary rapidly away from the centre. The peak compositions of both (a) and (b) arrangements is 1.64 and 1.62 at.% respectively.

For an arrangement comprising nine pieces of the second components, shown in Figure 4, there is a good improvement on the composition distribution. In Figure 4(b) where the nine chips were placed along the two surface diagonals of the target, it could be seen that the distribution is more uniform and the peaks do not so much deviate from the compositions of the other sections of the films. In Figure 4(a) however, in which the chips were arranged along the horizontal and vertical axes of the target surface, the distribution is much poorer in uniformity. The peaks occur around the central area of the atom flux and so much dwarf the composition at the neighbouring area.

The effects of anisotropy in the distribution of sputtered atoms are shown in Figure 5. When the second component is considered to be made up of Molybdenum which as he anisotropy function [4].

$$A_{Mo}(\psi)=1-0\cdot 132\psi+0\cdot 831\psi^2-0\cdot 172\psi^3-0\cdot 185\psi^4 \qquad (3.1)$$

the distribution of the three chips arrangement is shown in Figure 5(a). This when compared with the distribution depicted in (b) of the same figure, when the second component is thought to compose of Silicon atoms with the anisotropy [4]

$$A_si(\psi)=1\cdot 224+0\cdot 074\psi-0\cdot 413\psi^2+0\cdot 711\psi^3-0\cdot 388\psi^4 \qquad (3.2)$$

is less uniform with large isolated peaks.

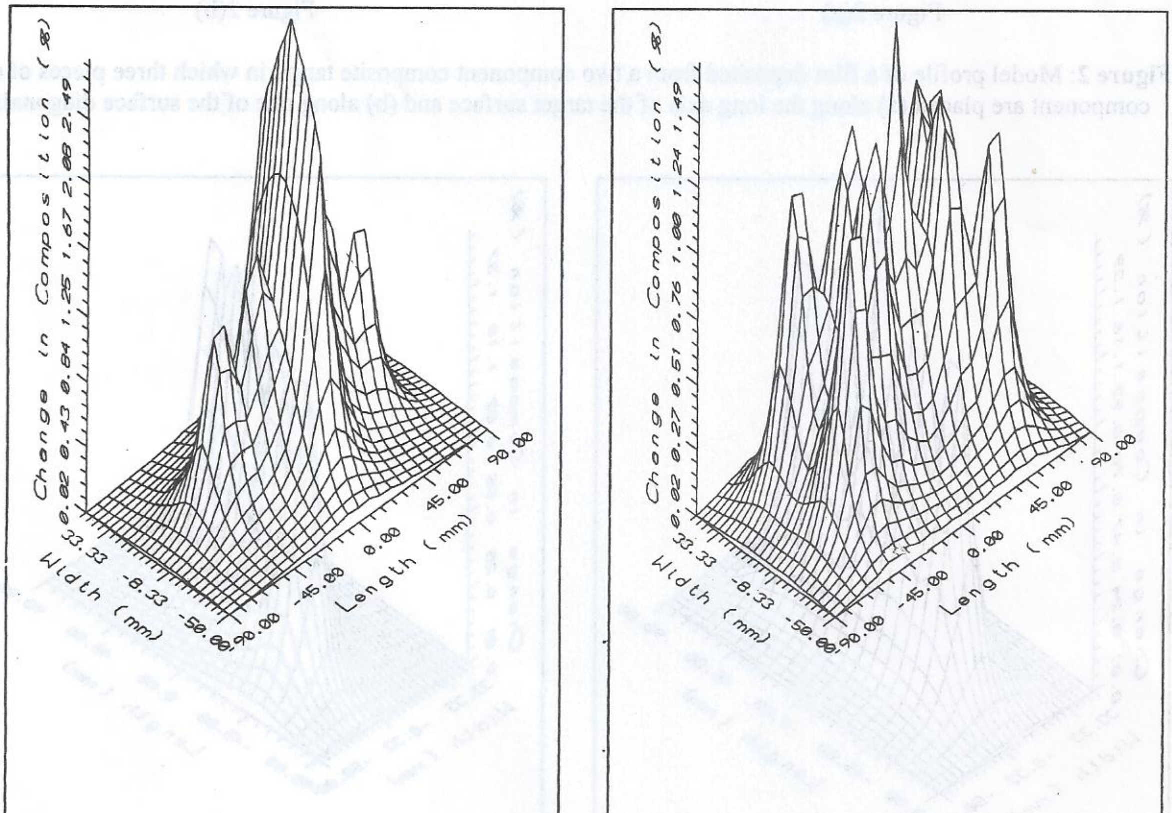

Figure 4(a) Figure 4(b)

Figure 4: Model profile of a film deposited from a two components composite target in which nine pieces of one component are placed (a) along the horizontal and the vertical axis of the target surface and (b) along the two surface diagonals.

4.0 Conclusion

The numerical simulation of the compositional distribution of the film does indicate that insightful information could be gained from the exercise. It is also observed that, while the total area of the target covered by the chips determine the expected composition of the chip material in the film, using smaller area chips lead to

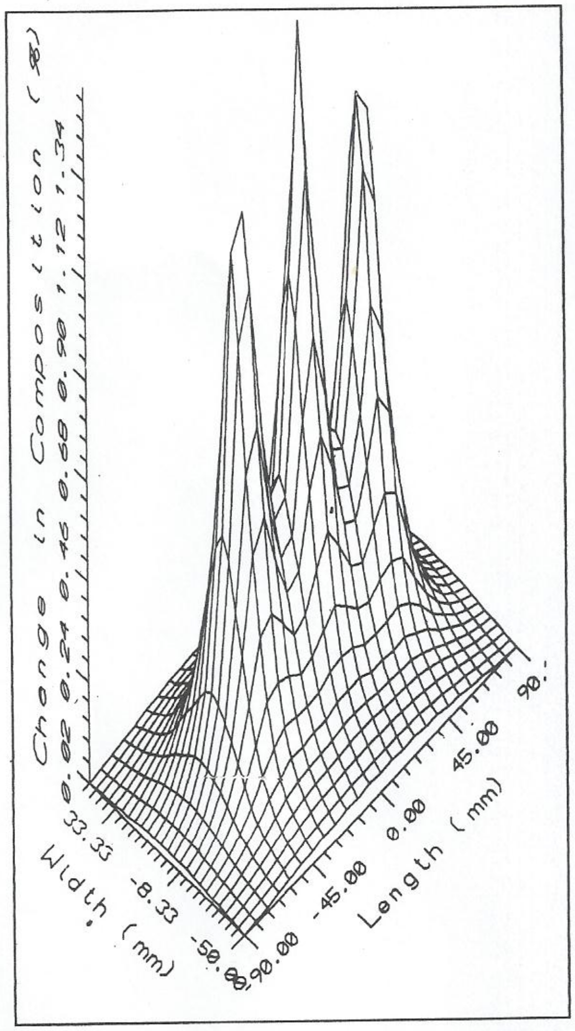

Figure 5(a)

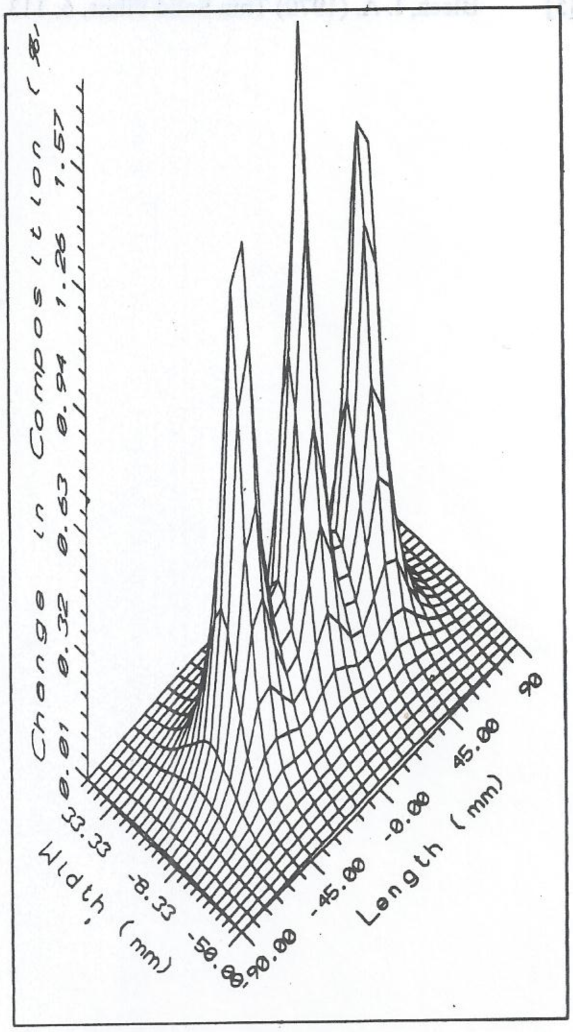

Figure 5(b)

Figure 5: Model profile of a film deposited from a two component composite target in which three pieces of one component are placed on the target surface (a) The angular distribution function of Mo is used and (b) that of Si is employed.

more uniform – that is more compositionally homogeneous films than using fewer but larger area chips. The manner of chip placement on the target also provided another avenue of controlling the uniformity. Lastly, the study did not take into consideration the possibility of the re-sputtering of the film surface. This and other related processes when studied might give better insight.

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