Manufacturability of highly doped Aluminum Nitride films

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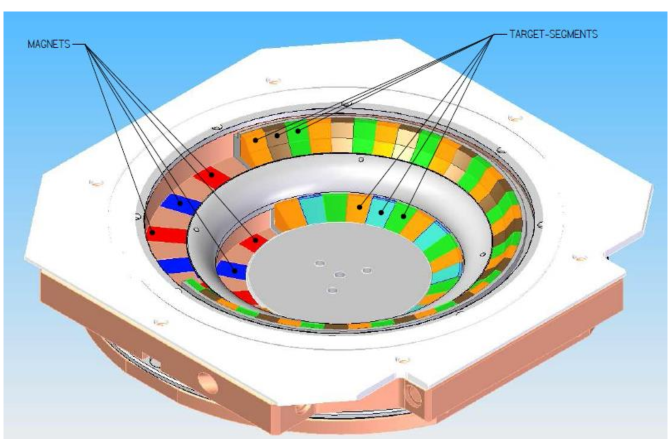
Abstract—There have been several investigations [1], [2], [3], that demonstrated benefits of adding dopants such as (Sc) or combination of other materials, like Zr/Mg for example, to the aluminum nitride (AlN) films in order to increase coupling coefficient (kt^2) of the Bulk Acoustic Wave (BAW) devices. For concentrations below 10% atomic Sc, it is possible to use a single composite target with a standard magnetron design [4]. Most R&D systems that performed initial investigations on AlScN films with high concentration of Sc dopant, used two separate targets with two separate magnetrons: one with pure Al and one with pure Sc with different applying power to compensate for the large difference in sputtering rates of the two materials and get stoichiometric composition. Unfortunately, depositing from two different targets is only viable for low volume R&D experiments. The system described in this article uses standard dual conical magnetron with AC deposition source. Targets are cut into multiple segments as shown in Figure 1 [5].

Figure 1. Multiple material targets



Based on simple geometry of target's surface, deposited film composition is proportional to the surface of specific pieces of target material. Unfortunately, Al is eroded at much higher rate than Sc at the same potential and same magnetic field. Over the target life, concentration of Sc increases in the deposited films. In order to maintain same Sc composition over the entire target life, it is necessary to vary magnetic field locally over the surface of the Al and Sc pieces to provide same erosion rate of Al vs. Sc at the same target potential. Adjusting magnetic field for each segment of both Al and Sc allows for constant deposited film composition over the entire target life solves this problem.

I. INTRODUCTION

Most PVD deposition processes that require multiple materials in a sputtering target use a composite target. Although it works well for most materials, some composite targets are extremely difficult to manufacture or even impossible. Also, they are very expensive. Binary Al/Sc targets are notoriously difficult to manufacture at Sc compositions above 10%. Theoretical maximum Sc concentration in aluminum with stable FCC crystal structure is about 22%, see Al-Sc phase diagram on figure 2 and table 1 and 2. However, the crystallographic texture should be remained relatively stable, retaining the preferred orientation ratios for good uniformity and stoichiometry during sputtering. Orientation ratios, compared to grain size, are the more critical parameter for sputtered film properties.

The AlSc phase diagram below shows the Al-Al3Sc eutectic reaction at very high temperature [6]. This process causes hot cracking of composite material, which were observed as black spots even below 10% of scandium composition in aluminum target. Higher Sc composition in Al target produces even worse problems.

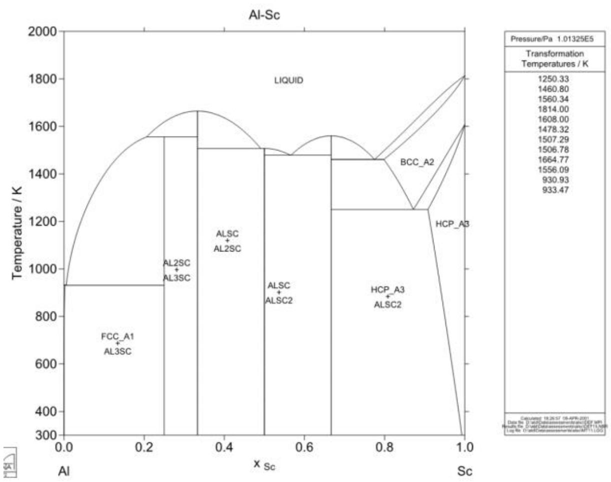
Table 1. Al-Sc Lattice parameter data

Phase	Composition, at.% Sc	Lattice parameters, nm a	c	Reference
Al	0	0.40496	...	[Massalski2]
Al_3Sc	25	0.4103	...	[65Mor]
Al_2Sc	33.3	0.7582	...	[74Mac]
AlSc	50	0.3450	...	[65Sch]
$AlSc_2$	66.7	0.4888	0.6166	[69Eym]
βSc	100	0.4541	...	[86Gsc]
αSc	100	0.33088	0.52680	[86Gsc]

Table 2. Al-Sc Crystal Structure data

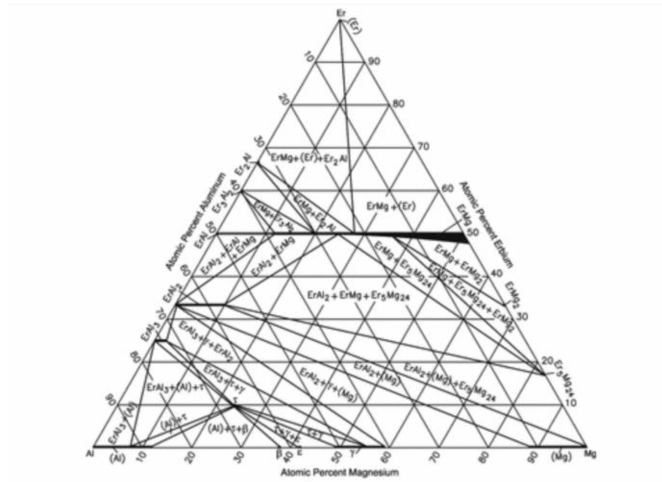
Phase	Composition, at.% Sc	Pearson symbol	Space group	Strukturbericht designation	Prototype	Reference
(Al)	0 to 0.38	$cF4$	$Fm\bar{3}m$	$A1$	Cu	[Pearson3]
Al_3Sc	25	$cP4$	$Pm\bar{3}m$	$L1_2$	$AuCu_3$	[65Mor]
Al_2Sc	33.3	$cF24$	$Fd\bar{3}m$	$C15$	Cu_2Mg	[74Mac]
AlSc	50	$cP2$	$Pm\bar{3}m$	$B2$	CsCl	[65Sch]
$AlSc_2$	66.7	$hP6$	$P6_3/mmc$	$B8_2$	Ni_2In	[69Eym]
(βSc)	~96 to 100	$cI2$	$Im\bar{3}m$	$A2$	W	[86Gsc]
(αSc)	~96 to 100	$hP2$	$P6_3/mmc$	$A3$	Mg	[86Gsc]

Figure 2. Calculated Al-Sc phase diagram



Composite Targets with three different materials, such as ternary compounds Al-Er-Mg or Al-Zr-Mg, are even more difficult to make. For example, Al-Er-Mg alloy may show multiple intermediate phases [7], [8], which results unstable properties of the deposited film.

Figure 3. Al-Er-Mg ternary compound phase diagram



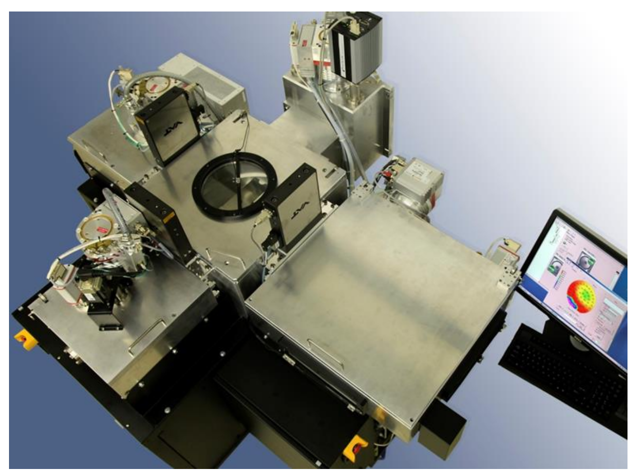
On other hand, sputtering from multiple targets from different magnetrons is not practical for high volume production due to low deposition rate and poor film thickness uniformity.

In this investigation we used multiple piece targets to produce highly piezoelectric films with Al, Sc, Mg and Er materials.

II. EQUIPMENT

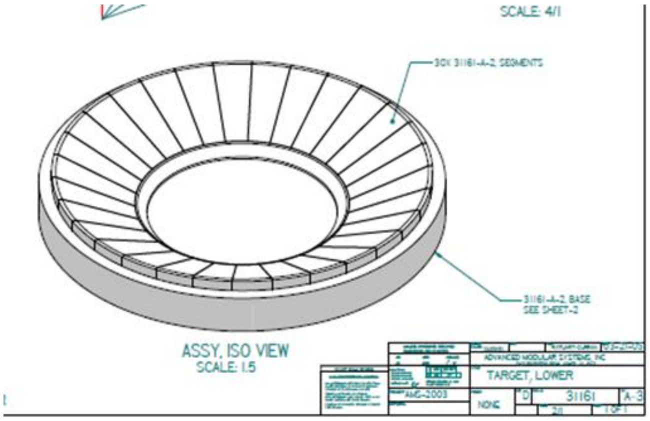
In this investigation we used Advanced Modular Systems cluster tool with AlN deposition chambers and ion beam trimming module (shown in Figure 4).

Figure 4. AMSystems cluster tool



AlN deposition uses a dual magnetron system with positive plasma column and with AC power applied between targets. Frequency of AC power is 40 kHz and power may vary from 3 to 10 kW. It is a reactive deposition process in deep poison mode using targets composed of Al and Sc pieces (tiles), see figure 5.

Figure 5. Multiple material targets



High purity research grade 99.9999% argon and nitrogen process gasses we used for all depositions.

Substrate rotation is using to compensate variation of scattering for different materials and composition non-uniformity across the substrate.

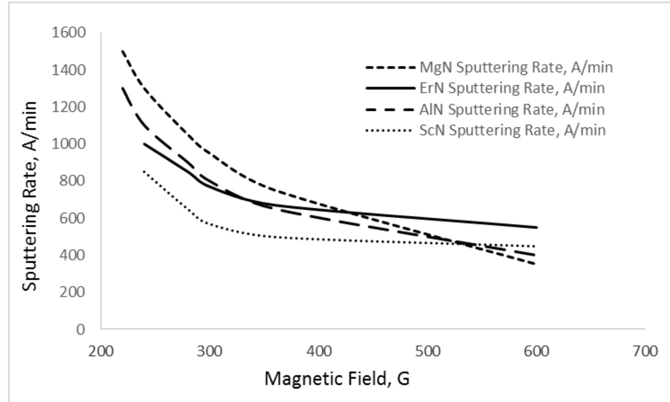
The trimming module uses DC focused ion source with argon process gas to improve thickness/uniformity of deposited films. Film thickness trimming/tuning is processing based on ion beam scanning across a wafer with power variation based on film thickness map. Use of the trimming process opens up a much wider process window for stress and composition control, because it allows avoiding of spending too much effort on controlling thickness uniformity during deposition.

III. Film Composition control

The system uses standard dual conical magnetron with AC deposition source. Targets are cut into multiple pieces/tiles as shown in Figure 5. Films containing various concentrations Scandium (Sc) and Erbium (Er) in AlSc(x)Er(y)N films, Scandium and Magnesium in AlSc(x)Mg(y)N films or Scandium in Al(x)Sc(y)N films have been demonstrated using different number of Sc and/or Er, or Sc and Mg pieces compare to the number of the Al pieces. As sputtering area of specific material increases, composition of this material in deposited film also becomes higher.

But not only pieces/tiles sputtering area effects on film composition. Sputtering rate of specific material has a very significant effect on film composition. Typically, for example, concentration of Sc in the AlScN film is about 66% of what it is in the deposition target with either composite targets or targets made out of pieces. It is much more obvious on the targets made out pieces of Al and Sc, that erosion of Al piece is significantly higher than the erosion of the adjacent Sc piece, if the same magnetic field is used. Sputtering rate for different material vs. magnetron magnetic field is shown below on figure 6.

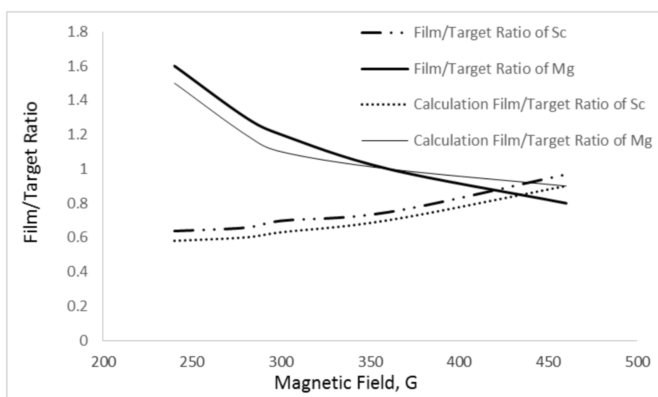
Figure 6. Sputtering Rate vs. Magnetron Magnetic Field



It is clear, that for Al-Sc deposition, for example, a constant magnetic field across of the magnetron will produce lower scandium composition film on the wafer than on the target if standard AlN magnetron is using. Changing the local magnetic field on the surface of tiles/segments with different sputtered materials results higher or lower concentration of desire dopant and a uniform target race track. We found that if we produce the same erosion of the Al and Sc targets, we get the same composition of Sc on the wafers as on the target. Based on Sputtering rate vs Magnetic field, we calculated compositions of different dopant's concentration in AlN film depends on concentration of the same dopant in the target.

For Al-Sc deposition, increasing magnetic field on the surface of the aluminum pieces, increases Sc composition on the deposited film on the substrate, but it produces opposite result for Al-Mg deposition, as shown in figure 7.

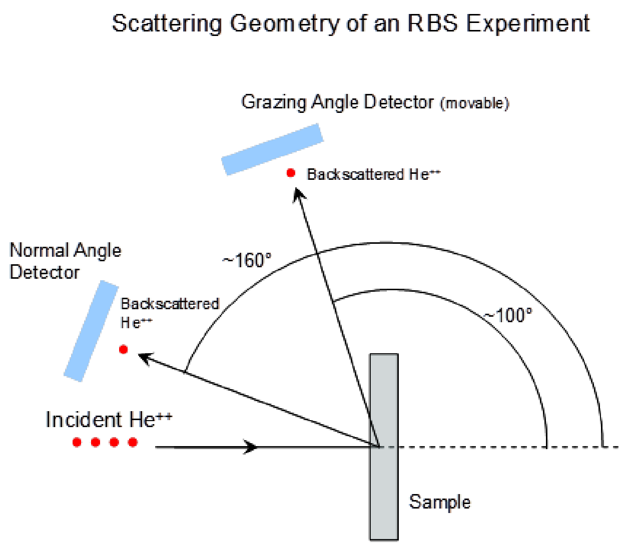
Figure 7. Film/Target Ratio of Composition of Sc and Mg as a function of the magnetic field at the Al pieces



Some mismatch between calculated and actual film/target composition ratio versus magnetic field could be considered as an error for different scattering shape for different type of dopant (heavier atoms, normally at given target voltage, have broader scattering and some material is losing due to deposition on shields. Lighter atoms, at given target voltage, have, usually, more narrow scattering and more material reaches a substrate). Also, we didn't consider smooth variation of magnetic field from tile/piece to tile/piece. Since magnetic field has continuous (smooth) function, and we can't produce it as a step function.

Film's compositions were measured by Rutherford Backscattering Spectrometry. Rutherford Backscattering Spectrometry spectra are acquired at a backscattering angle of 160° and an appropriate grazing angle (with the sample oriented perpendicular to the incident ion beam). The schematic diagram below shows the scattering geometry in a typical RBS experiments.

Figure 8. Scattering Geometry of an Rutherford Backscattering Spectrometry Experiments



Uniformity of sputtering rate changes over the target life. Fortunately Sc or Mg concentration across wafer and over the target life doesn't change appreciably. This allows for a robust production process that can easily be fixed by ion beam trimming. Figures 9, 10 and 11 below, show AlScN deposited film properties over the target life, including thickness uniformity with parallel trimming process, with adjusted local magnetic field for Al and Sc tiles/pieces.

Figure 9. Film stress of AlScN deposition as a function of target life

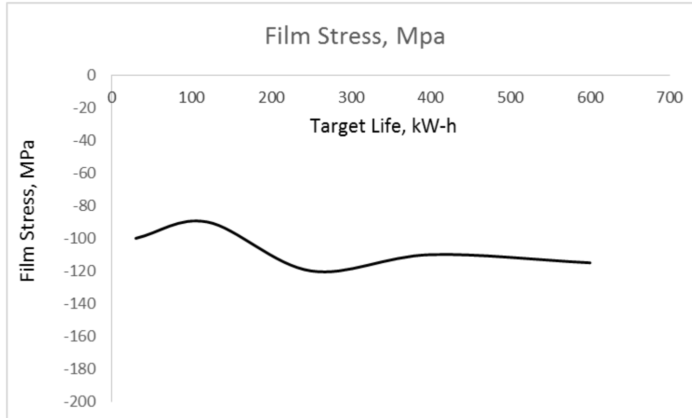


Figure 10. Film uniformity of AlScN deposition as a function of target life

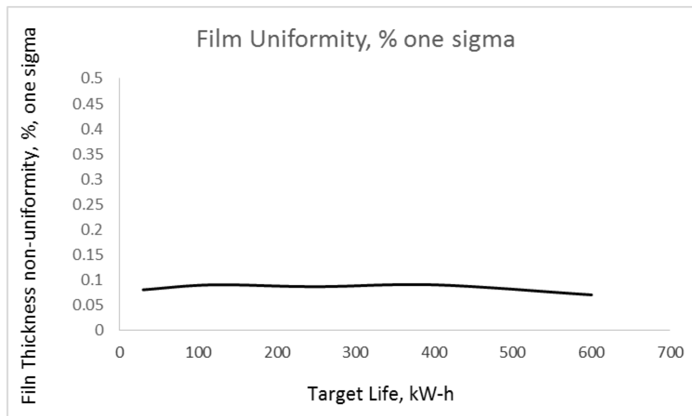
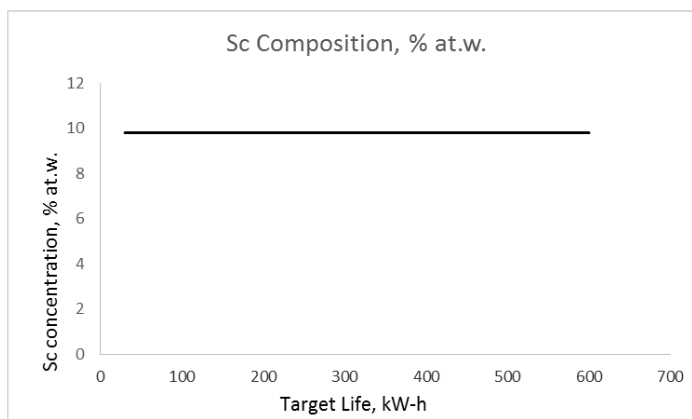


Figure 11. Film properties of AlScN deposition as a function of target life



IV. SUMMARY

Using custom and local adjusted magnetic field and thickness trimming, we were able to demonstrate production worthy highly doped AlN deposition process.

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