# Epitaxial growth of Solid State Ionics Materials

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Epitaxial thin films of materials used in solid state ionics like Yttrium Stabilized Zirconia (YSZ), Rare Earth Oxides (REO) are suitable systems to study the interfacial ion transport. YSZ is an efficient oxygen ion conductor, vacancy present are responsible for ionic transport. By altering the structure we can increase the ionic conductivity. An attempt was made to computationally mock the sputtering process and deposit these films and study the diffusion of the adatom on the surface. There exists a strong interaction of the ions formed in the plasma during the sputtering process, the adatoms and the sputtering parameters which also affects the final device performance which can be batteries, solid oxide fuel cell (SOFC), ionic membranes, sensors or ceramic oxygen generators (COG). Introduction of gases for reactive sputtering also complicates the system.

Keywords: Epitaxial, YSZ, REO, sputtering, ion conductivity

The rate of deposition of $ZrO_2$ at 600 eV Ar ion bombardment is 40 Å/s. Yttrium on the other hand has a sputtering rate of 85 Å/s in the same condition [3]. For the YSZ thin film we will consider the slower rate of deposition i.e 40 Å/s . The atomic radii of Zr is 206 pm and that if Y is 212 pm. As the film is mainly $ZrO_2$ with Y as additive we will consider 206 pm for atomic layer calculation. The Atomic layers were calculated for 1 s to 100 s. The deposition rate shows abrupt changes with oxygen flow rates [4].

We must understand that the rate of sputtering and rate of deposition are two different parameters. The adatoms of from the target will be acted upon by oxygen to get finally deposited. The oxide formation therefore usually takes place during the traversing of adatoms from source to the target.

Going backwards as per our proposed model, we can estimate the rate of sputtering from the rate of deposition which comes out to be same as the rate of deposition. Thus the change is deposition rate is due to oxygen flow and its reaction with the adatoms after they have been ejected out from the target.

The sputtering rate of the compound material formed by reaction of oxygen introduced in the sputtering chamber with the target is much less than that of target itself. The target is also called poisoned target which has been dealt by us previously while modeling sputter deposition of TiOx films [5]. A change in phase is reported due to oxygen flow rate difference during sputtering where also a sharp transition in deposition rate is observed [6].

The variation of atomic layers of $ZrO_2$ deposited with rate of sputtering varying from 10 to 100 Å/s is shown in Fig 1

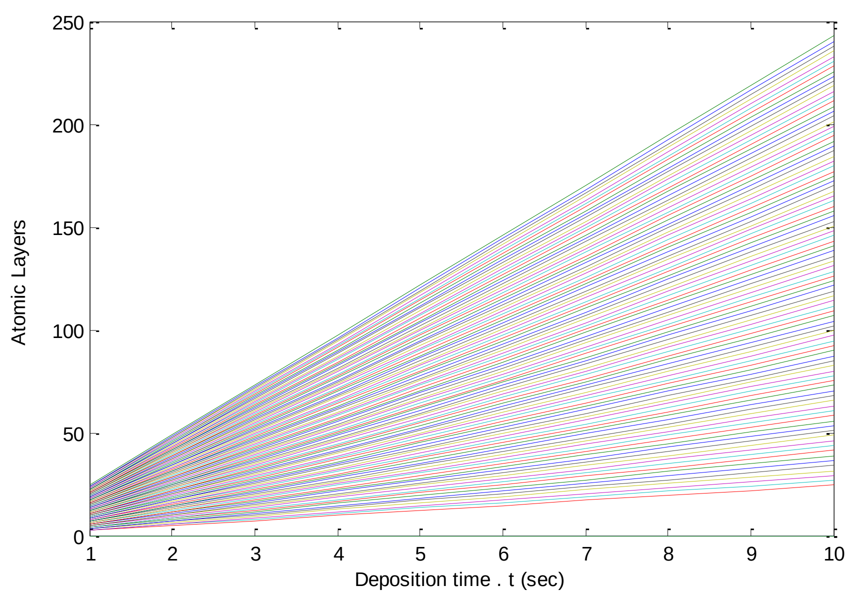


Fig 1 : Atomic layers deposited of $ZrO_2$ with rate of sputtering varying from 10 to 100 Å/s

As proposed in ref [6] the rate is almost halved suddenly when there is oxide formation we assume a change of rate from 80 Å/s to 40 Å/s. The sputter rate of element Zr is 85 Å/s which confirms this fact. A linear variation of Atomic Layers of Zr with deposition time is shown in Fig 2.

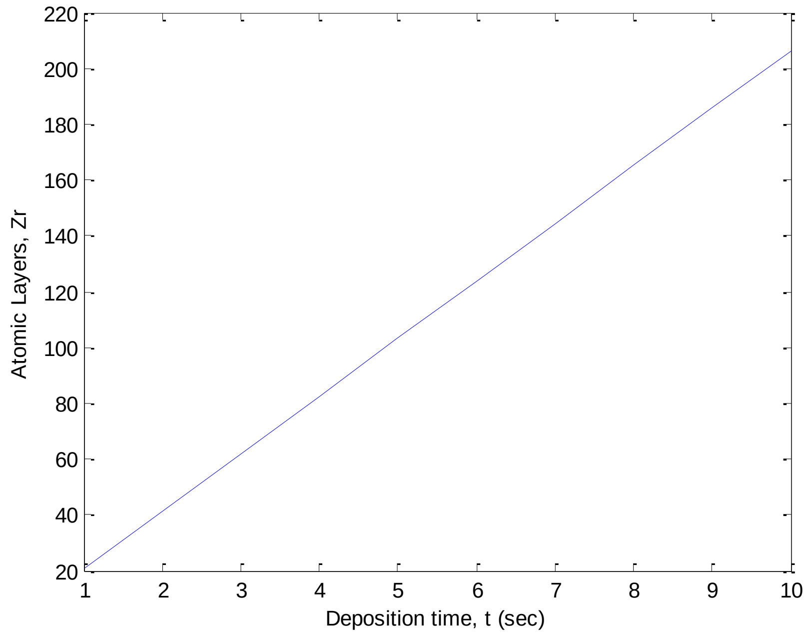


Fig 2 Linear variation of Atomic Layers of Zr with deposition time

The difference between Atomic layers of Zr and ZrO2 is the effect of oxygen flow. The variation of atomic layers difference with deposition time and its derivative giving the oxygen deposition rate is shown in Fig 3.

Interestingly instead of one abrupt change as reported before, we are observing here more than one abrupt changes. Foe now we can say that the sudden decrease corresponds to oxide adsorption and desorption of oxygen on the surface. The variation has an oscillatory nature as shown in Fig 4.

The results show that there exists a strong interaction of the ions formed in the plasma during the sputtering process and the adatoms as well as reactive gases introduced. The phenomenon of adsorption and surface diffusion needs in this case needs to be looked into.

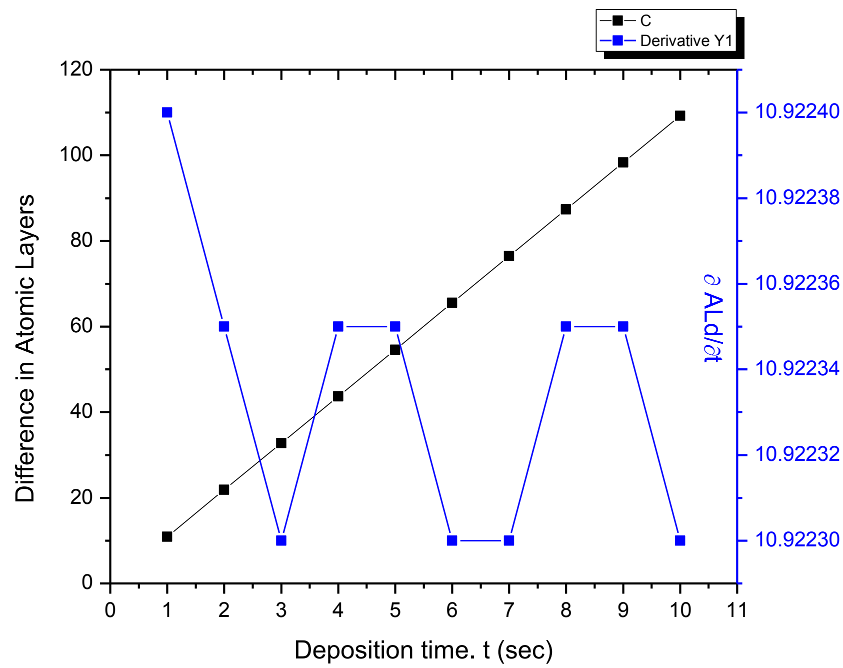


Fig 3 : Variation of atomic layers difference with deposition time and its derivative

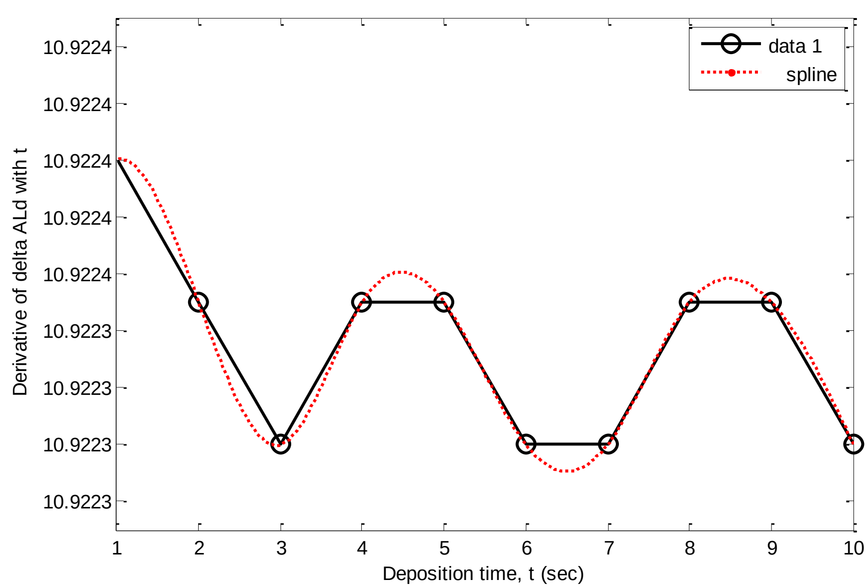


Fig 4: Oscillatory nature of the variation of derivative of atomic layers difference w.r.t deposition time

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## MATLAB Codes

```
rZr=2.06;
for zt = 10:10:100;
for t=1:10;
AL (t,zt) =t*zt/(2*rZr);
x=0.3;
k=1.4e-23;
T=300;
L=k*T;
ALdZrO2=AL*exp(-x\L);
end
end

rZr=2.06;
zt =85;
t=1:10;
AL=t*zt/(2*rZr);
x=0.3;
k=1.4e-23;
T=300;
L=k*T;
ALd=AL*exp(-x\L);
ALd=ALd';

DAL=ALd-ALdZrO2(:,40);
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