Incorporation of magnesium into ZnMgO layers grown by PA-MBE.

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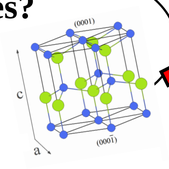
Why ZnO/ZnMgO structures?

- Wide direct band gap 3.37eV to 4.0eV (at 300K)
- Large 60 meV exciton binding energy (ZnO)
- Stable excitonic emission at room temperature
- Cheaper alternative to GaN
- Compatible with GaN due to its crystal symmetry, large exciton binding energy and large band gap comparable
- Excellent candidate for use in visible and ultraviolet light emitters and detectors.



What do we want to show?

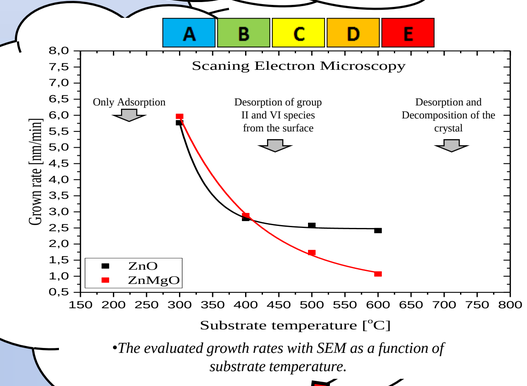
- The aim of our work is to investigate influence of substrate temperature on incorporation of magnesium into ZnMgO layers grown by PA-MBE.

How to show it?

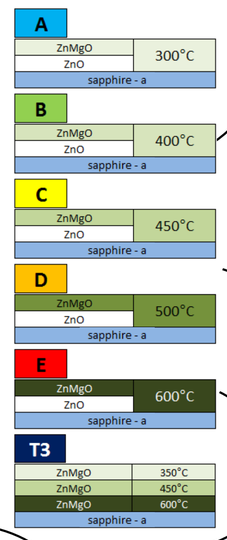
- Make a set of ZnO/ZnMgO layers by MBE at the same growth conditions but at different substrate temperature.
- Estimate Mg content in ZnMgO layers by Photoluminescence and X-Ray Diffraction.

What structures were made?

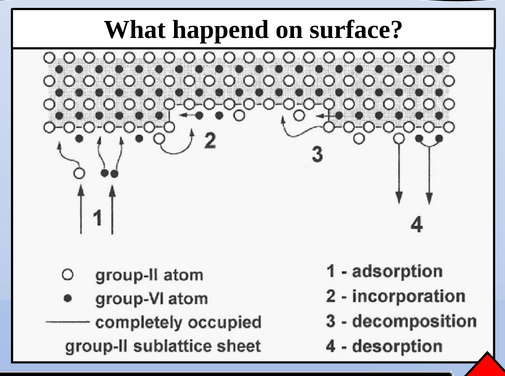
What about growth rate?



•The evaluated growth rates with SEM as a function of substrate temperature.

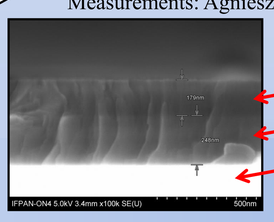


What happend on surface?

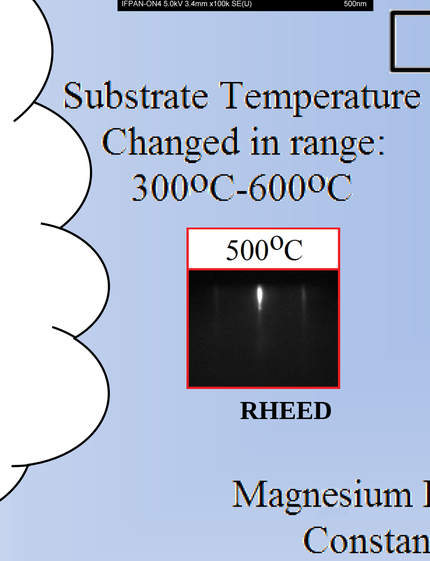


Scaning Electron Microscopy

Measurements: Agnieszka Pieniążek



Why concentration of Mg in ZnMgO layers rise with substrate temperature?



RHEED

How to check whether ZnO decomposition takes place?

The decomposition rate of ZnO in vacuum can be measured in the same way as in work: *N. Grandjean, Appl. Phys. Lett. 74, 1854.* To estimate the decomposition rate below equation was used:

$$V_d = \frac{\beta}{\alpha} V_g$$

N. Grandjean, Appl. Phys. Lett. 74,1854

In the range of temperatures used in our case, the decomposition rate is neglegtable ~0.05 nm/min.

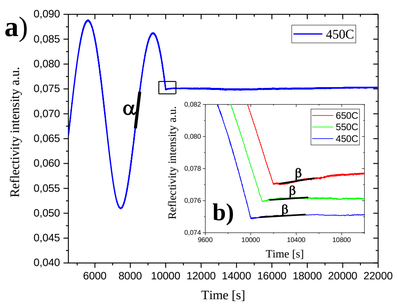
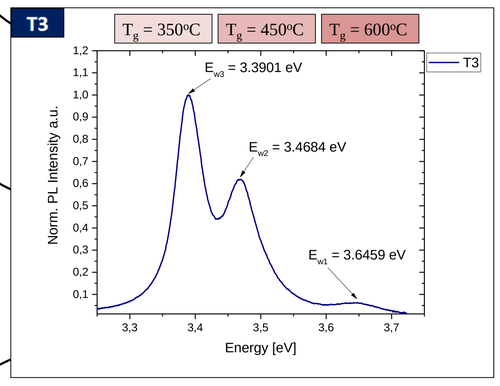


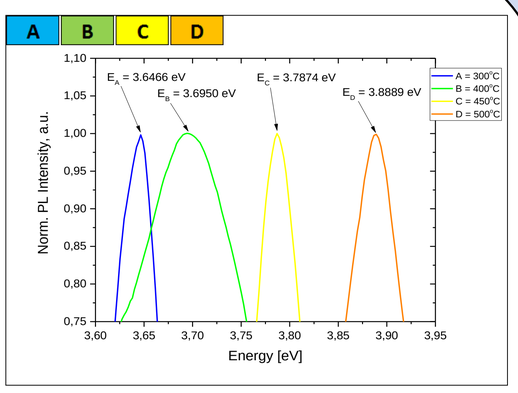
*Fig. a) Reflectivity intensity oscillations recorded during growth of ZnO at 450°C. b) Reflectivity intensity variation during evaporation of ZnO in vacuum as a function substrate temperature. The slopes **α** and **β** are proportional to the growth rate and to the evaporation rate, respectively.*

What are the evidence for the influence of substrate temperature on Mg concentration in ZnMgO layers?

Photoluminescence



• Photoluminescence spectra for ZnMgO thin films at 10 K.



• Photoluminescence spectra for ZnMgO thin films at 10 K.

		Temp. [°C]	Energy [eV]	Composition of Mg [%]
T3	w1	600	3,6459	**18,93**
	w2	450	3,4684	**7,18**
	w3	350	3,3901	**1,99**
A		300	3,6466	**18,98**
B		400	3,695	**22,19**
C		450	3,7874	**28,30**
D		500	3,8889	**35,03**
E		600	?	**?**

We used the following equation to estimate the composition of Mg in $Zn_{1-x}Mg_xO$ layers:

$$E_{PL} = 1{,}51x + 3{,}36eV$$

The above equation is a fit to the results of PL, where precise determination of the Mg concentration x was performed by elastic recoil detection analysis ERD:

B. Laumer, et. al., J. Appl. Phys. 133, 233512(2013)

How to explain evolution of growth rates as a function of substrate temperature?

- Perhaps by Sticking Coefficient.

$$Sc = \frac{N_{ads}}{N_{tot}}$$

The sticking coefficient is defined as the ratio of the number of atoms adsorbed, or "sticked", to the substrate surface to the total number of atoms that impinge upon the substrate surface during the same period of time.

A Sc for Oxygen is independent of substrate temperature but a Sc for metal elements is inversely proportional to the exponential of the temperature and also inversely proportional to the square of the distance between atomic steps on the surface of a crystalline material.

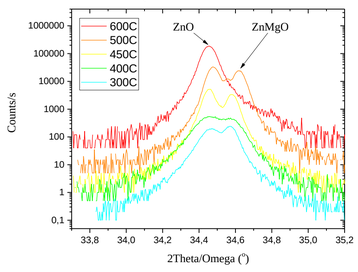
X-Ray Diffraction

The composition of magnesium calculated from the Vegard's law:

$$x_c = \frac{c(x_c)_{ZnMgO} - c_{ZnO}}{c_{MgO} - c_{ZnO}} * 100\%$$

Ref . Schleife A, Fuchs F, Furthmuller J, Bechstedt F 2006 *Phys. Rev.* B **73** 245212

$$C_{MgO} = 5.136A$$

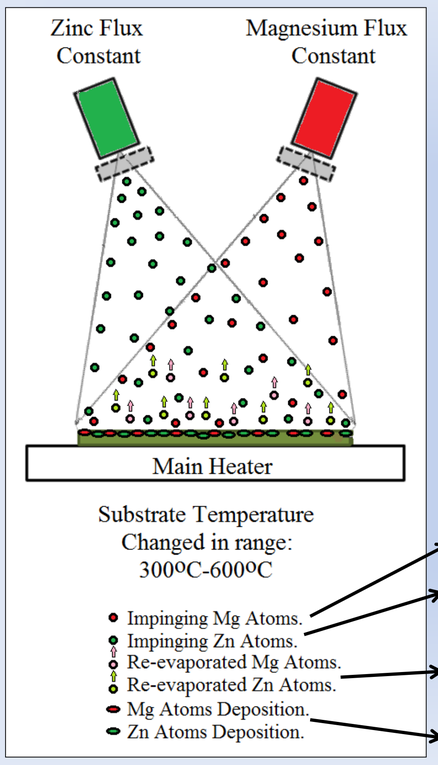


• X-ray diffraction 2Θ/ω scans of 00.2 ZnO/ZnMgO symmetrical reflection of ZnO/ZnMgO epitaxial layers on a-plane sapphire.

	Temp. [°C]	C [A]	Composition of Mg [%]
A	300	5,1857	**20,35**
B	400	5,1847	**21,96**
C	450	5,1831	**25,12**
D	500	5,1779	**33,39**
E	600	?	**?**

Discussion

The composition variation in the alloys as a function of the growth temperature can be explained by the difference of vapor pressure between Mg and Zn elements at high growth temperatures. Due to the higher saturation pressure of Zn vapor, Zn atoms can be easily re-evaporated at higher growth temperature yielding Mg enriched films. Effectively, higher Mg concentration in the alloy films are obtained when grown at higher temperatures.



Impinging Atoms $Mg = \frac{FluxMg}{M_{A_{Mg}} * 10000cm^2}$

Impinging Atoms $Zn = \frac{FluxZn}{M_{A_{Zn}} * 10000cm^2}$

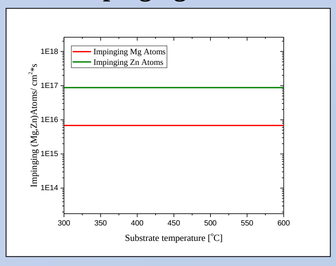
Re-evaporated Atoms $= W_n * \frac{p(i)}{[2\pi M(i)RT]^{\frac{1}{2}}} * N_A$

R.H. Lamoreaux, J.Phys.Chem. 16, 3 (1987)

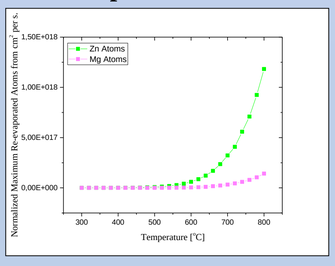
(Mg, Zn) Deposition Atoms = Impinging Atoms (Mg, Zn) – Re-evaporated Atoms (Mg, Zn)

Where:
Flux Zn [Pa/s] Flux Mg [Pa/s]
M_{AZn} Zn atomic Mass [kg].
M_{AMg} Mg atomic Mass [kg].
M(*i*) and p(*i*) are gram-molecular weight and equilibrium partial pressure of vapor species *i*, and R and T are the molar gas constant and absolute temperature. N_A is the Avogadro constant.
W_n - normalization factor.

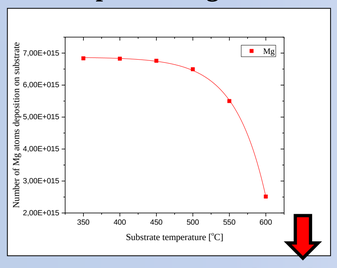
What about Impinging Atoms?



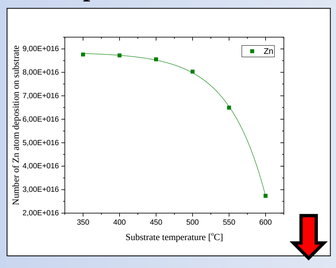
What about Re-evaporation Atoms?



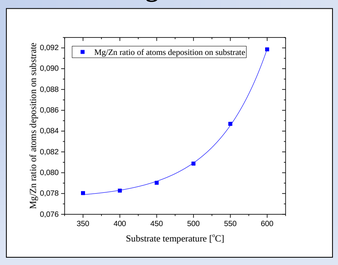
What about Deposited Mg Atoms?



What about Deposited Zn Atoms?



What about Mg/Zn Atom Ratio?



Summary:

- **The MBE $Zn_{1-x}Mg_xO$ and ZnO layers were characterised with various techniques (RHEED, Laser Reflection Interferometry, PL, XRD, SEM) to estimate their optical and structural properties.**
- **XRD and PL measurements allowed to calculate the Mg content in the ZnMgO layers. The results obtained with different techniques are consistent.**
- **The influence of the substrate temperature on the Mg concentration is evident and well documented.**
- **The increased concentration of Mg at higher substrate temperatures is caused by different (higher) desorption coefficient of Zn to Mg.**

Acknowledgement :

This work was partly supported by the Polish National Science Centre (NCN) Grant No. 2014/13/B/St7/01773