

# DiethylZinc (Precursor for ZnO thin film deposition in Atomic Layer Deposition)

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# Overview

- Experimental Procedure
- Literature survey:
  - Mechanism of ZnO thin film deposition in ALD
  - Chemical and Structural Characterization of ALD-ZnO films
- MSDS information about chemical
- Operating procedure for chemical usage

# Experimental procedure

- RCA cleaning of Si wafer
- Deposition of ZnO on Si wafer by ALD

Precursors for reaction:

Metal Precursor: DiethylZinc ( $\text{Zn}(\text{C}_2\text{H}_5)_2$ )

Oxidizing Agent: DI Water ( $\text{H}_2\text{O}$ )

Substrate Temperature range: 100-300 °C

- Al metal contact deposition by an evaporation process in a Au contaminated tool, followed by characterization.

# Mechanism of ZnO thin film Deposition in ALD

- Chemical reaction:



This reaction occurs in two stage, when the half-part chemical reactions take place at the surface during DEZn (phase 1) and water (phase 2) pulses.

Assume a substrate surface terminated by hydroxides (-OH)

- DEZn phase:  $\text{surface-OH} + \text{C}_2\text{H}_5\text{-Zn-C}_2\text{H}_5 \rightarrow \text{surface-O-Zn-C}_2\text{H}_5 + \text{C}_2\text{H}_6$

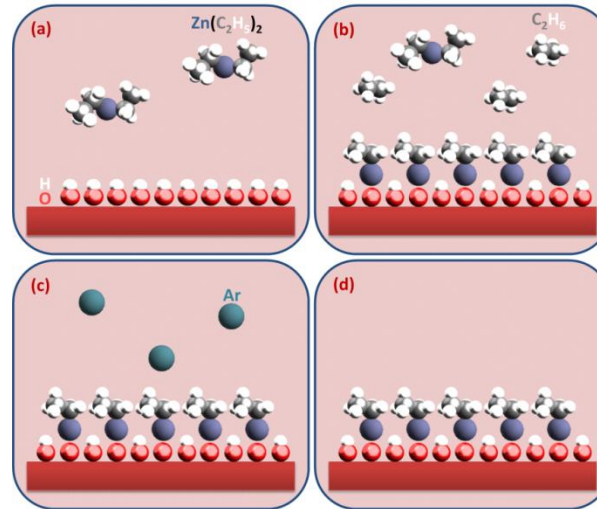


Figure 1: Reaction mechanism of the first ALD half-reaction using diethylzinc and water to form ZnO. (a) DEZn exposure; (b) ligand exchange; (c) Ar purge; (d) monoethylzinc saturated surface.

- Water phase:  $\text{surface-O-Zn-C}_2\text{H}_5 + \text{H}_2\text{O} \rightarrow \text{surface-O-Zn-OH} + \text{C}_2\text{H}_6$

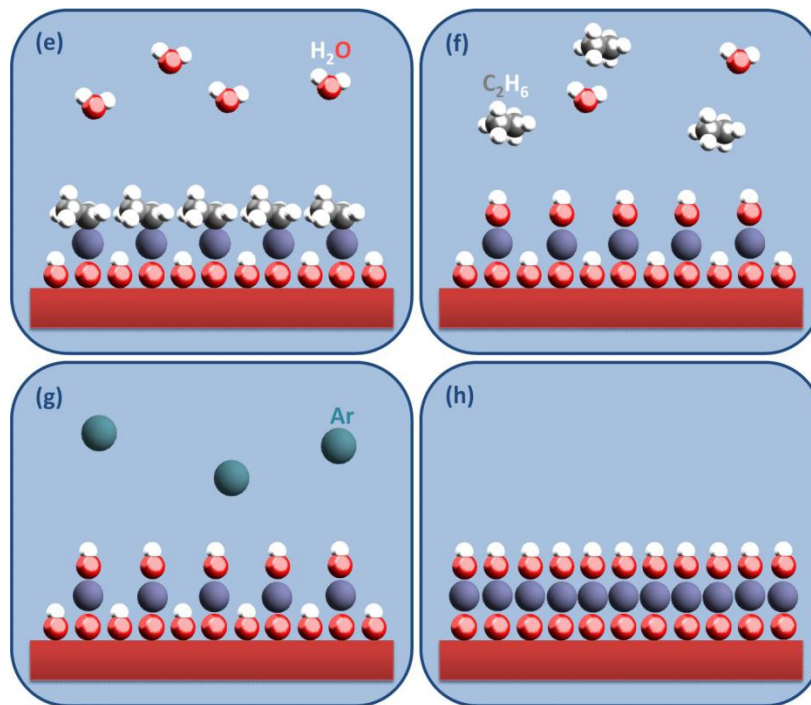


Figure 2: Reaction mechanism of the second ALD half-reaction using diethylzinc and water to form ZnO. (e)H<sub>2</sub>O exposure; (f) ligand exchange; (g) Ar purge; (h)hydroxide saturated ZnO monolayer.

# Chemical and Structural Characterization of ALD-ZnO films

- XPS of ZnO thin film on Si(111):

After background removal, peak fitting results reveal a [Zn]:[O] ratio of 0.97, i.e. the ZnO layer is close to the stoichiometric composition of 1.00. Also the Auger parameters were calculated which revealed that ALD has the ability to deposit ZnO layers .

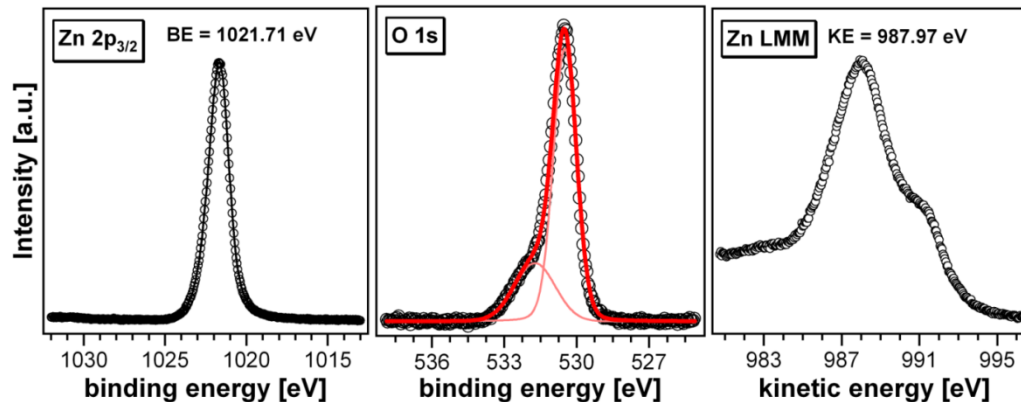


Figure 3: Photoemission spectra of an ALD-ZnO layer much thicker than the escape depth of the photoelectrons. All spectra are recorded using Al-K $\alpha$  radiation of 1486.7 eV. Quantification of the spectra results in a [Zn]:[O] ratio of 0.97 and a zinc Auger parameter of 2009.68 eV.

- XRD data of ZnO thin film on Si(111) by ALD:

Data shows the prominent (002) reflection peak which refers that ZnO is growing in wurtzite structure.

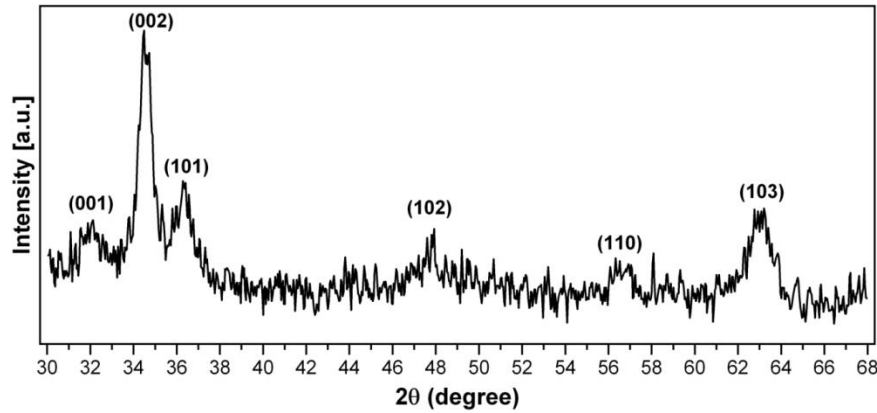


Figure 4: Grazing-incidence X-ray diraction data of an approx. 50 nm thick ALD ZnO layer.

## Conclusion:

- Literature survey shows the evidence of formation of ZnO thin film by ALD.

## Reference:

- Doctoral Theisis by Eike Janocha from Technical University of Berlin, Faculty IV – Electrotechnology and Computer science. Guided by Prof. Dr. Bernd Rech, Prof. Dr. Christian Pettenkofer, Prof. Dr. Wolfgang Jäger. Berlin 2012.

# MSDS

## HANDLING AND STORAGE:

- Precautions for safe handling:
  1. Avoid inhalation of vapour or mist.
  2. Use explosion-proof equipment. Keep away from sources of ignition - No smoking. Take measures to prevent the build up of electrostatic charge.
- Conditions for safe storage:
  1. Keep container tightly closed in a dry and well-ventilated place. Containers which are opened must be carefully resealed and kept upright to prevent leakage.
  2. Never allow product to get in contact with water during storage.
  3. Air sensitive



## DISPOSAL CONSIDERATIONS:

- Product

Burn in a chemical incinerator equipped with an afterburner and scrubber but exert extra care in igniting as this material is highly flammable. Offer surplus and non-recyclable solutions to a licensed disposal company. Contact a licensed professional waste disposal service to dispose of this material.

- Contaminated packaging

Dispose of as unused product.

# Operating procedure for chemical usage

- **Detailed procedure of usage:**

Training will be provided by vendor for

- Handling the precursors in the system.
- To load a cylinder
- To pump out head space (air)
- To remove the cylinder
- Also tips on determining usage, how much precursor is left and make suggestions on how to store and handle empty cylinders.
- The end over products will be pumped out by a exhaust.

- Will method of usage release any decomposition/ oxidizing products:

- Area in which chemical will be used: I Floor

- Equipment where chemical is used: ALD

- Users list, mail id's and cell numbers:

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- **Usage timing:**

- **Access to fire extinguisher-phone**